

A hierarchical extension scheme for backward solutions of the Wright–Fisher model

Julian Hofrichter, Tat Dat Tran, Jürgen Jost

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We develop an iterative global solution scheme for the backward Kolmogorov equation of the diffusion approximation of the Wright-Fisher model of population genetics. That model describes the random genetic drift of several alleles at the same locus in a population from a backward perspective. The key of our scheme is to connect the solutions before and after the loss of an allele. Whereas in an approach via stochastic processes or partial differential equations, such a loss of an allele leads to a boundary singularity, from a biological or geometric perspective, this is a natural process that can be analyzed in detail. A clarification of the role of the boundary resolves certain uniqueness issues and elucidates the construction of hierarchical solutions.

Keywords: Wright-Fisher model; random genetic drift; backward Kolmogorov equation; global solution; loss of alleles

1 Introduction

The most basic mechanism of mathematical population genetics is random genetic drift. Parents are randomly chosen from the current generation and transfer the alleles that they possess at some genetic locus to their offspring. The process is repeated over many generations, and once an allele gets lost from the population because at the current step no carrier of that allele is chosen as a parent, it will be lost forever from the population. Thus, in the end, at each locus, only a single allele will survive. This then leads to questions like the chances of the different alleles present in the initial population to be the survivor, or the expected times of the allele losses, and so on. In order to start an investigation of such questions, Fisher [12] and Wright [38] developed the most basic model. In that model, there is a finite population of finite size N which is kept across the generations. Time is discrete, and each time step, the parental generation is replaced by an offspring generation. That offspring generation is formed by random sampling with replacement. Mathematically speaking, this means that each of the N individuals in the

offspring generation randomly and independently chooses a parent. As each individual has only a single parent, no recombination takes place. Each individual carries a single locus. At this locus, each individual carries one of $n+1$ possible alleles labelled $0, 1, \dots, n$. Initially, the population possesses n different alleles for that locus. There are no selective differences between those alleles, and no mutations occur.

Of course, the model can be and has been generalized, to several loci, recombination, mutations, selective differences etc., see [11, 4] for recent textbooks on mathematical population genetics. Nevertheless, the original model remains of considerable mathematical interest, and the issues around the loss of allele events contain some subtle mathematical structure. And that is what we shall focus upon in the present paper. Generalizations along the lines just indicated will then be presented elsewhere.

The mathematical investigation of the Wright-Fisher model owes much to the pioneering work of Kimura [21, 22, 23]. A crucial step was not to work with the original model of a finite population evolving in discrete time steps, but with the diffusion approximation for an infinite population in continuous time. This then leads to the forward and backward Kolmogorov equations. The forward equation is a partial differential equation of parabolic type, whereas the backward equation, the adjoint of the former w. r. t. a suitable product, evolves backward in time and therefore is not parabolic. Mathematical difficulties arise from the fact that both equations become degenerate at the boundary. In this paper, we shall investigate the boundary behavior of the Kolmogorov backward equation, that is

$$-\frac{\partial}{\partial t}u(p, t) = \frac{1}{2} \sum_{i,j=1}^n p^i(\delta_j^i - p^j) \frac{\partial^2}{\partial p^i \partial p^j} u(p, t) =: L_n^* u(p, t), \quad (1.1)$$

where p^i is the relative frequency of allele i ; p^0 does not appear in (1.1) because of the normalization $\sum_{i=0}^n p^i = 1$. One readily sees that coefficients become 0 when one of the frequencies p^i becomes 0. Since we are working in the closure of the probability simplex $\Delta_n = \{(p^1, \dots, p^n) : p^i > 0, \sum_{j=1}^n p^j < 1\}$, this means that the PDE (1.1) becomes degenerate at the boundary of Δ_n . (The fact that (1.1) is not parabolic because time is running backward is not such a serious problem, because of the structure of the model and the duality with the – parabolic – Kolmogorov forward equation.)

The Kolmogorov equations have been studied with tools from the theory of stochastic processes, see for instance [7, 9, 10, 20], and from the theory of partial differential equations [5, 6]. These approaches, because of their general nature, yield certain existence, uniqueness and regularity results, but cannot come up with explicit formulas, for instance for the expected time of loss of an allele. Therefore, other authors focused on the specific and explicit structure of the model. Among many other things, the global aspect, that is, connecting the solutions in the interior of the simplex and on its boundary faces, has been addressed in the literature, and a number of representation formulas has been derived. There is some discussion in Section 5.10 of [11], as well as in [4], but we wish to describe some of the relevant results in more detail and with a different focus.

The first solution schemes for the Kolmogorov equations were of a local nature. In 1956, Kimura solved the Kolmogorov forward equation for the 3-allelic case ($n = 2$)

in [24]. Baxter, Blythe and McKane in [3] solved the case of an arbitrary number of alleles by separation of variables. And in fact, the Kolmogorov backward equation also always has simple global stationary solutions (cf. section 10). The main achievement of this paper will be to compile the existing local solutions into a non-trivial global solution by handling the boundary singularities.

In the literature, using an observation of [30], one usually writes the Kolmogorov backward operator in the form

$$\Lambda_n^* u(x, t) := \frac{1}{2} \sum_{i,j=0}^n x^i (\delta_j^i - x^j) \frac{\partial^2}{\partial x^i \partial x^j} u(x, t), \quad (1.2)$$

using the variables (x^0, x^1, \dots, x^n) with $\sum_{j=0}^n x^j = 1$ in place of $L_n^* u(p, t)$ (cf. equation (1.1)) with (p^1, \dots, p^n) and $p^0 = 1 - \sum_{i=1}^n p^i$ implicitly determined (for our notation, see Sections 2 and 3, in particular (2.1) and (3.2)), that is, one works on the simplex $\{x^0 + x^1 + \dots + x^n = 1, x^i \geq 0\}$, i.e., the variable x^0 is included. This has the advantage of being symmetric w.r.t. all x^i , but the disadvantage that the operator invokes more independent variables than the dimension of the space on which it is defined. In other words, the elliptic operator becomes degenerate. In our treatment, we have opted to work with L_n^* , but for the comparison with the literature, we shall utilize the version (1.2).

The starting point of much of the literature to be referenced here is the observation of Wright [39] that when one includes mutation, the degeneracy at the boundary is removed. More precisely, let the mutation rate m_{ij} be the probability that when allele i is selected for offspring, the offspring carries the mutant j instead of i . One also puts $m_{ii} = -\sum_{j \neq i} m_{ij}$. The corresponding Kolmogorov backward operator then becomes

$$\Lambda_n^* u(x, t) := \frac{1}{2} \sum_{i,j=0}^n x^i (\delta_j^i - x^j) \frac{\partial^2}{\partial x^i \partial x^j} u(x, t) + \sum_{j=0}^n \sum_{i=0}^n m_{ij} x^i \frac{\partial}{\partial x^j}. \quad (1.3)$$

Wright [39] then discovered that a mathematically very convenient assumption is

$$m_{ij} = \frac{1}{2} \mu_j > 0 \text{ for } i \neq j, \quad (1.4)$$

that is, the mutation rates only depend on the target gene (the factor $\frac{1}{2}$ is inserted solely for purposes of normalization) and are positive. With (1.4), (1.3) becomes

$$\Lambda_n^* u(x, t) := \frac{1}{2} \sum_{i,j=0}^n x^i (\delta_j^i - x^j) \frac{\partial^2}{\partial x^i \partial x^j} u(x, t) + \frac{1}{2} \sum_{j=0}^n (\mu_j - \sum_{i=0}^n \mu_i) x^j \frac{\partial}{\partial x^j}. \quad (1.5)$$

In this case, the Wright-Fisher diffusion has a unique stationary distribution, given by the Dirichlet distribution with parameters μ_0, \dots, μ_n . A further simplification occurs when

$$\mu_0 = \dots = \mu_n =: \mu > 0, \quad (1.6)$$

that is, when all mutation rates are the same. The assumption (1.4) that the mutation rates only depend on the target gene is not so natural biologically (the mutation rate should rather depend on the initial instead of the target gene, but (1.6) remedies that deficit in a certain sense), but for our purposes the more crucial issue is the assumption of positivity.

Several papers have studied this model and derived explicit formulas for the transition density of the process with generator (1.5); they include [27, 31, 13, 14, 32, 33, 8, 15]. A powerful tool in this line of research has been Kingman's coalescent [25], that is, the method of tracing lines of descent back into the past and analyzing their merging patterns (for a quick introduction to that theory, see also [19]). In particular, some of these formulas also apply in the limiting case $\mu = 0$ in (1.6). Ethier-Griffiths [8] showed that the following formula for the transition density

$$P(t, x, dy) = \sum_{M \geq 1} d_M^0(t) \sum_{|\alpha|=M, \alpha \in \mathbb{Z}_+^n} \binom{|\alpha|}{\alpha} x^\alpha \text{Dir}(\alpha, dy), \quad (1.7)$$

which had earlier been derived under the assumption $\mu > 0$, pertains to the case $\mu = 0$. Here, Dir is the Dirichlet distribution, and $d_M^0(t)$ is the number of equivalence classes of lines of descent of length M at time t in Kingman's coalescent for which analytical formulas have been derived in [33]. (1.7) has been studied further in many subsequent papers, for instance [15]. Shimakura [32] has the less explicit formula

$$\begin{aligned} P(t, x, dy) &= \sum_{m \geq 1} e^{-\lambda_m t} E_m(x, dy) \\ &= \sum_{K \in \Pi} P(t, x, y) dS_K(y) \\ &= \sum_{K \in \Pi} e^{-\lambda_m t} E_{m,K}(x, y) dS_K(y). \end{aligned} \quad (1.8)$$

Here, the λ_m are the eigenvalues introduced above, and E_m stands for the projection onto the corresponding eigenspace, and the index K enumerates the faces of the simplex. The Dirichlet distribution in (1.7) and the measure $dS_K(y)$ in (1.8) both become singular when y approaches the boundary of K . The point here is that the sum invokes solutions on the individual faces, and the transition from one face into one of its boundary faces becomes singular in this scheme. In fact, (1.8) is simply a decomposition into the various modes of the solutions of a linear PDE, summed over all faces of the simplex.

In this paper, we want to get a more detailed analytical picture of the behavior at the boundary and develop a global solution on the entire state space including its stratified boundary. In an important recent work, Epstein and Mazzeo [5, 6] have developed PDE techniques to address the issue of solving PDEs on a manifold with corners that degenerate at the boundary with the same leading terms as the Kolmogorov backward equation for the Wright-Fisher model

$$-\frac{\partial}{\partial t} u(p, t) + L_n^* u(p, t) = f, \quad (1.9)$$

in the closure of the probability simplex in $(\overline{\Delta}_n)_{-\infty} = \overline{\Delta}_n \times (-\infty, 0)$ (see also lemma 3.3). These results apply to a rather wide class of such PDEs. An important part of their work is the identification of appropriate function spaces. In our context, their spaces $C_{WF}^{k,\gamma}(\overline{\Delta}_n)$ would consist of k times differentiable functions whose k th derivatives are Hölder continuous with exponent γ w.r.t. the Fisher metric. (This only holds true for L_n^* , although E&M also use this construction for their generalised setting.) In terms of the Euclidean metric on the simplex, this means that a weaker Hölder exponent (essentially $\frac{\gamma}{2}$) is required in the normal than in the tangential directions at the boundary. They then show that when the right hand side f of (1.9) is of class $C_{WF}^{k,\gamma}(\overline{\Delta}_n)$ for some $k \geq 0, 0 < \gamma < 1$, and if the initial values are of class $C_{WF}^{k,2+\gamma}(\overline{\Delta}_n)$ (essentially C^{k+2} with a suitable Hölder condition on k th, $(k+1)$ th and scaled $(k+2)$ th derivatives), then there exists a unique solution in that latter class. This result is very satisfactory from the perspective of PDE theory (see e.g. [18]). Here, however, we are considering solutions that are not even continuous, let alone of some class $C^{0,2+\gamma}(\overline{\Delta}_n)$, as we want to study the boundary transitions (nevertheless, there are some points of contact in section 10). Therefore, in this paper, we carry out a detailed investigation of the boundary behavior of solutions of (1.9). A particular issue is the relation between several loss of allele events that can occur in different possible orders. In analytical terms, the issue is the regularity of solutions at singularities of the boundary, that is, where two or more faces of the simplex Δ_n meet. We also consider particular extension paths from the boundary into the interior of the simplex. They have nothing to do, however, with Kingman's coalescent lines of descent as utilized in some of the literature discussed above. Kingman's scheme is concerned with tracing common ancestors of members of the current population of alleles. In contrast to that, we are interested in the directions in which the singularities of the boundary of the simplex are approached from the interior, because we are interested in the continuity at the boundary.

In contrast to the approaches discussed above that invoke strong tools from the theory of stochastic processes, our approach is not stochastic, but analytic and geometric in nature. In that sense, our approach is closer in spirit to that of [5, 6]. In contrast to that approach, however, we develop geometric constructions, within the framework of information geometry, that is, the geometry of probability distributions, see [1, 2], in order to have an approach that on one hand is naturally capable of studying such generalizations as indicated above, but on the other hand can still derive explicit formulas. This is part of a general research program, see [34, 16, 35, 36, 37, 17]. The present paper, which is based on [16], is the backward counterpart to [17], which investigated the Kolmogorov forward equation.

The solutions of the backward Kolmogorov equation are the probability distribution over ancestral states yielding some given current state of allele frequencies. Thus, time runs backward, indeed, as the name indicates. Such an ancestral state could have possessed more alleles than the current state, because on the path towards that latter state, some alleles that had been originally present in the population could have been lost. In analytical terms, one could assume that such a loss of allele event is continuous, in the sense that the relative frequency of the corresponding allele simply goes to 0. Geomet-

rically, however, this means that the process moves from the interior of a probability simplex into some boundary stratum and henceforth stays there. Also, when two or more alleles got lost, they could have disappeared in different orders from the population. The main achievement of the current paper then is a global and hierarchical solution for the Kolmogorov backward equation that persists and stays regular across different such loss of allele events in the past. This is technically rather involved and has not been achieved before in the literature. For a complete understanding and a rigorous solution of the Kolmogorov backward equation, however, this is indispensable. Of course, one needs to know how many alleles there had been in the original population, or equivalently, how many alleles got lost between the ancestral and the current state of the populations.

Here is a more precise description of the content of this paper. We face the issue of the degeneracy at the boundary of the Kolmogorov equations head on. Although creating analytical difficulties, biologically and geometrically, this is very natural because it corresponds to the loss by random drift of some alleles from the population in finite time. As mentioned above, this has to happen almost surely. After an allele gets lost, the population keeps evolving by random genetic drift. The Wright-Fisher process has to be applied with fewer alleles than before, but otherwise there is no conceptual difference. Of course, the process stops when only one allele is left. Therefore, it is biologically essential and geometrically natural to connect the processes before and after the loss of an allele.

In the current backward setting, the perspective of an allele loss is reversed: A process with, say, n alleles taking place on an $(n - 1)$ -dimensional probability simplex, may originate from a process with $n + 1$ alleles on an n -dimensional simplex by loss of an allele. The former then should be identified as a facet of the latter, that is, the loss of an allele simply means that the process moves from the interior into the boundary of the simplex of subsequent higher dimension from. Of course, this will be repeated backwards, incorporating the previous loss of further alleles. Thus, the process could have originated from higher and higher dimensional simplices until its ultimate starting configuration. In this paper, we therefore construct a global solution that incorporates and connects these successive loss of allele events. In technical terms, we develop a hierarchical scheme that relies on a careful analysis of the connection modes and tailored regularity specifications for the corresponding solutions.

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2 Preliminaries and notation

We consider a population that initially carries $n+1$ different alleles at a single locus. The allele distribution of the next generation is chosen by random sampling with replacement from the current generation. In other words, we repeatedly sample a binomial distribution. As pioneered by Kimura, we consider the diffusion approximation of the process, where we let the population size $N \rightarrow \infty$ and rescale the discrete generation time as $t = \frac{1}{N}$. This leads to the Kolmogorov equations for the evolution of the probability distribution of the alleles. In contrast to the population size, the number of alleles is kept finite. Therefore, as we are interested in the relative allele frequencies, the state space is the n -dimensional probability simplex.

In this section, we shall recall the notation from [17] that is necessary for the iterative transition to boundary strata of this simplex within a hierarchical scheme, as well as the appropriate function spaces.

p^0, p^1, \dots, p^n denote the relative frequencies of alleles $0, 1, \dots, n$. Because of $\sum_{j=0}^n p^j = 1$, we have $p^0 = 1 - \sum_{i=1}^n p^i$.

$$\Delta_n := \left\{ (p^1, \dots, p^n) \in \mathbb{R}^n \mid p^i > 0 \text{ for } i = 1, \dots, n \text{ and } \sum_{i=1}^n p^i < 1 \right\}, \quad (2.1)$$

is the (open) n -dimensional standard orthogonal simplex. Equivalently, we have

$$\Delta_n = \left\{ (p^0, \dots, p^n) \in \mathbb{R}^{n+1} \mid p^j > 0 \text{ for } j = 0, 1, \dots, n \text{ and } \sum_{j=0}^n p^j = 1 \right\}. \quad (2.2)$$

The topological closure of this simplex is

$$\overline{\Delta}_n = \left\{ (p^1, \dots, p^n) \in \mathbb{R}^n \mid p^i \geq 0 \text{ for } i = 1, \dots, n \text{ and } \sum_{i=1}^n p^i \leq 1 \right\}. \quad (2.3)$$

Time is $t \in (-\infty, 0]$, and

$$(\Delta_n)_{-\infty} := \Delta_n \times (-\infty, 0).$$

The subsimplices in the boundary $\partial\Delta_n = \overline{\Delta}_n \setminus \Delta_n$ are called *faces*, from the $(n-1)$ -dimensional *facets* down to the 0-dimensional *vertices*. Each subsimplex of dimension $k \leq n-1$ is isomorphic to the k -dimensional standard orthogonal simplex Δ_k . For an index set $I_k = \{i_0, i_1, \dots, i_k\} \subset \{0, \dots, n\}$ with $i_j \neq i_l$ for $j \neq l$, we put

$$\Delta_k^{(I_k)} := \left\{ (p^1, \dots, p^n) \in \overline{\Delta}_n \mid p^i > 0 \text{ for } i \in I_k; p^i = 0 \text{ for } i \in I_n \setminus I_k \right\}. \quad (2.4)$$

In particular, $\Delta_n = \Delta_n^{(I_n)}$.

Each of the $\binom{n+1}{k+1}$ subsets I_k of I_n corresponds to a boundary face $\Delta_k^{(I_k)}$ ($k \leq n-1$). The k -dimensional part of the boundary $\partial_k \Delta_n$ of Δ_n is therefore

$$\partial_k \Delta_n^{(I_n)} := \bigcup_{I_k \subset I_n} \Delta_k^{(I_k)} \subset \partial \Delta_n^{(I_n)} \quad \text{for } 0 \leq k \leq n-1. \quad (2.5)$$

Formal consistency thus also leads to $\partial_n \Delta_n = \Delta_n$. This boundary concept can be iteratively applied to simplices in the boundary of some $\Delta_l^{(I_l)}$, $I_l \subset I_n$ for $0 \leq k < l \leq n$. This means that

$$\partial_k \Delta_l^{(I_l)} = \bigcup_{I_k \subset I_l} \Delta_k^{(I_k)} \subset \partial \Delta_l^{(I_l)}. \quad (2.6)$$

The simplex $\Delta_k^{(\{i_0, \dots, i_k\})}$ represents the state where the $k+1$ alleles i_0, \dots, i_k are present in the population, and $\partial_k \Delta_n$, that is, the union of all those simplices, represents the state where the number of alleles is $k+1$, but where their identity does not matter. When any one of the alleles i_0, \dots, i_k is eliminated, we land in $\partial_{k-1} \Delta_k^{(\{i_0, \dots, i_k\})}$.

We next introduce spaces of square integrable functions for our subsequent integral products on Δ_n and its faces (which will be used implicitly, for details cf. [36]),

$$L^2\left(\bigcup_{k=0}^n \partial_k \Delta_n\right) := \left\{ f: \overline{\Delta_n} \longrightarrow \mathbb{R} \mid f|_{\partial_k \Delta_n} \text{ is } \mathbb{A}_k\text{-measurable and} \right. \\ \left. \int_{\partial_k \Delta_n} |f(p)|^2 \mathbb{A}_k(dp) < \infty \text{ for all } k = 0, \dots, n \right\}. \quad (2.7)$$

Here, \mathbb{A}_k stands for the k -dimensional Lebesgue measure, but when integrating over some $\Delta_k^{(I_k)}$ with $0 \notin I_k$, the measure needs to be replaced with the one induced on $\Delta_k^{(I_k)}$ by the Lebesgue measure of the containing \mathbb{R}^{k+1} – this measure, however, will still be denoted by \mathbb{A}_k as it is clear from the domain of integration $\Delta_k^{(I_k)}$ with either $0 \in I_k$ or $0 \notin I_k$ which version is actually used. In particular, for the top-dimensional simplex, we simply have

$$L^2(\Delta_n) := \left\{ f: \Delta_n \longrightarrow \mathbb{R} \mid f \text{ is } \mathbb{A}_n\text{-measurable and } \int_{\Delta_n} |f(p)|^2 \mathbb{A}_n(dp) < \infty \right\}. \quad (2.8)$$

We also need spaces of k times continuously differentiable functions, for $k \in \mathbb{N} \cup \{\infty\}$,

$$C_0^k(\overline{\Delta_n}) := \{f \in C^k(\overline{\Delta_n}) \mid f|_{\partial \Delta_n} = 0\}, \quad (2.9)$$

$$C_0^k(\Delta_n) := \{f \in C^k(\Delta_n) \mid \exists \bar{f} \in C_0^k(\overline{\Delta_n}) \text{ with } \bar{f}|_{\Delta_n} = f\} \quad (2.10)$$

as well as

$$C_c^k(\overline{\Delta_n}) := \{f \in C^k(\overline{\Delta_n}) \mid \text{supp}(f) \subsetneq \Delta_n\}. \quad (2.11)$$

In order to define an extended solution on Δ_n and its faces (indicated by a capitalised U), we shall in addition need appropriate spaces of pathwise regular functions. Such a solution needs to be at least of class C^2 in every boundary instance (actually, a solution typically always is of class C^∞ , which likewise applies to each boundary instance). Moreover, it should stay regular at boundary transitions that reduce the dimension by one, i. e. for $\Delta_k^{(I_k)}$ and a boundary face $\Delta_{k-1} \subset \partial_{k-1} \Delta_k^{(I_k)}$. Globally, we may require

that such a property applies to all possible boundary transitions within $\overline{\Delta}_n$ and define correspondingly for $l \in \mathbb{N} \cup \{\infty\}$

$$U \in C_p^l(\overline{\Delta}_n) :\Leftrightarrow U|_{\Delta_d^{(I_d)} \cup \partial_{d-1}\Delta_d^{(I_d)}} \in C^l(\Delta_d^{(I_d)} \cup \partial_{d-1}\Delta_d^{(I_d)}) \quad \text{for all } I_d \subset I_n, 1 \leq d \leq n \quad (2.12)$$

with respect to the spatial variables. Likewise, for ascending chains of (sub-)simplices with a more specific boundary condition, we put for index sets $I_k \subset \dots \subset I_n$ and again for $l \in \mathbb{N} \cup \{\infty\}$

$$U \in C_{p_0}^l\left(\bigcup_{d=k}^n \Delta_d^{(I_d)}\right) :\Leftrightarrow \begin{cases} U|_{\Delta_d^{(I_d)}} \text{ is extendable to } \bar{U} \in C^l(\Delta_d^{(I_d)} \cup \partial_{d-1}\Delta_d^{(I_d)}) \text{ with} \\ \bar{U}|_{\partial_{d-1}\Delta_d^{(I_d)}} = U\chi_{\Delta_{d-1}^{(I_{d-1})}}\chi_{\{d>k\}} \text{ for all } \max(1, k) \leq d \leq n \end{cases} \quad (2.13)$$

with respect to the spatial variables. We note that such a function may straightforwardly be completed into a function defined on the entire $\overline{\Delta}_n$ by putting $U := 0$ on $\overline{\Delta}_n \setminus (\bigcup_{d=k}^n \Delta_d^{(I_d)})$ for corresponding t ; however, such an extension is generally not of class $C_p^l(\overline{\Delta}_n)$ w. r. t. the spatial variables.

3 The Kolmogorov operators

On an interior simplex Δ_n , the *Kolmogorov backward equation* for the diffusion approximation of an n -allelic 1-locus Wright–Fisher model reads

$$\begin{cases} -\frac{\partial}{\partial t}u(p, t) = L_n^*u(p, t) & \text{in } (\Delta_n)_{-\infty} = \Delta_n \times (-\infty, 0) \\ u(p, 0) = f(p) & \text{in } \Delta_n, f \in \mathcal{L}^2(\Delta_n) \end{cases} \quad (3.1)$$

for $u(\cdot, t) \in C^2(\Delta_n)$ for each fixed $t \in (-\infty, 0)$ and $u(p, \cdot) \in C^1((-\infty, 0))$ for each fixed $p \in \Delta_n$ and with the *backward operator*

$$L_n^*u(p, t) := \frac{1}{2} \sum_{i,j=1}^n (p^i(\delta_j^i - p^j)) \frac{\partial^2}{\partial p^i \partial p^j} u(p, t). \quad (3.2)$$

Analogously, we have

$$L_n u(p, t) := \frac{1}{2} \sum_{i,j=1}^n \frac{\partial^2}{\partial p^i \partial p^j} (p^i(\delta_j^i - p^j)u(p, t)) \quad (3.3)$$

being the *forward operator* appearing in the corresponding Kolmogorov forward equation. The definitions of the operators given in equations (3.3) and (3.2) also apply to the closure $\overline{\Delta}_n$; we point this out as we shall also consider extensions of the solution and the differential equation to the boundary.

For relations between the two operators, we immediately have the following lemmas; the corresponding proofs may be found in [17]:

3.1 Lemma. L_n and L_n^* are (formal) adjoints with respect to the product $(\cdot, \cdot)_n$ in the sense that

$$(L_n u, \varphi)_n = (u, L_n^* \varphi)_n \quad \text{for } u \in C^2(\overline{\Delta}_n), \varphi \in C_0^2(\overline{\Delta}_n). \quad (3.4)$$

3.2 Lemma. For an eigenfunction $\varphi \in C^2(\overline{\Delta}_n)$ of L_n and $\omega_n := \prod_{k=1}^n p^k (1 - \sum_{l=1}^n p^l)$, we have: $\omega_n \varphi \in C_0^2(\overline{\Delta}_n)$ is an eigenfunction of L_n^* corresponding to the same eigenvalue and conversely.

We continue with some further observations on the operators, in particular with regard to the boundary of Δ_n : The operator L_n^* , if restricted to subsimplices $\Delta_k^{(I_k)} \cong \Delta_k$ in $\partial\Delta_n^{(I_n)}$ of any dimension k , then again is the adjoint of the differential operator L_k corresponding to the evolution of a $(k+1)$ -allelic process in Δ_k :

3.3 Lemma. For $0 \leq k < n$ and $I_k \subset \{0, \dots, n\}$, $|I_k| = k$, we have

$$L_n^*|_{\Delta_k^{(I_k)}} = L_k^*. \quad (3.5)$$

We may therefore omit the index k in L_k^* whenever convenient, in particular when considering domains where (parts of) the boundary are included. For the operator L_n , we do not have such a restriction property.

The probabilistic interpretation is that the backward solution $u(p, t)$ expresses the probability of having started in some $p \in \Delta_n$ at the negative time t conditional upon being in a certain state $u(p, 0) = f(p)$ at time $t = 0$, i. e. having reached the corresponding (generalised) target set.

4 Solution schemes for the Kolmogorov backward equation

Solutions of the Kolmogorov backward equation and of the Kolmogorov forward equation are linked by the adjointness relation for the Kolmogorov operators L_n and L_n^* given in lemma 3.1, and hence known solution schemes (cf. [24], [3]) are essentially applicable for either equation. However, there is a subtle difference in the context of the non-matching spectra of L_n and L_n^* (cf. [36]): All eigenfunctions of L^* acquired by the adjointness relation in lemma 3.2 are in $C_0^\infty(\Delta_n)$, but L_n^* in Δ_n possesses even more eigenfunctions (in particular for smaller eigenvalues) since all eigenfunctions of L_k^* in Δ_k for some $0 \leq k < n$ also occur as eigenfunctions of L_n^* by e. g. constant extension.

With the eigenfunctions (e. g. the generalised Gegenbauer polynomials, cf. [34]) given, the construction of a solution of equation (3.1) in Δ_n is rather straightforward. However, the – in comparison with the forward case – larger set of eigenfunctions causes ambiguities when decomposing a final condition, which prevents uniqueness results for the solution. But if we restrict the choice of eigenfunctions to the ‘proper’ eigenfunctions in the domain¹, i. e. those in $C_0^\infty(\Delta_n)$, which are derived from eigenfunctions of L_n , the

¹This is also sufficient as their linear span is already dense in $C_c^\infty(\overline{\Delta}_n)$ and consequently also in $\mathcal{L}^2(\Delta_n)$: Linear combinations of the generalised Gegenbauer polynomials as eigenfunctions of L_n (cf. [34]) are dense in $C^\infty(\overline{\Delta}_n)$; dividing a function $f \in C_c^\infty(\overline{\Delta}_n)$ by ω_n (cf. lemma 3.2) again yields a function in $C_c^\infty(\overline{\Delta}_n) \subset C_0^\infty(\overline{\Delta}_n)$ as ω_n is in $C_0^\infty(\overline{\Delta}_n)$ itself and positive in the interior Δ_n .

existence and uniqueness of a solution observed in the forward case likewise apply. Thus, for such a solution by proper eigenfunctions (which will be called a *proper solution of the Kolmogorov backward equation in Δ_n*), we have, coinciding with the result of e. g. [27]:

4.1 Proposition. *For $n \in \mathbb{N}$ and a given final condition $f \in \mathcal{L}^2(\Delta_n)$, the Kolmogorov backward equation corresponding to the diffusion approximation of the n -dimensional Wright–Fisher model (3.1) always allows a unique proper solution $u: (\Delta_n)_{-\infty} \rightarrow \mathbb{R}$ with $u(\cdot, t) \in C_0^\infty(\Delta_n)$ for each fixed $t \in (-\infty, 0)$ and $u(p, \cdot) \in C^\infty((-\infty, 0))$ for each fixed $p \in \Delta_n$.*

By construction, proper solutions do not cover the boundary. In the next section, the non-proper components will be interpreted as originating from (proper) solutions on lower-dimensional boundary strata.

5 Inclusion of the boundary and the extended Kolmogorov backward equation

We shall now include the boundary and its contribution into the model. We augment the domain of equation (3.1) such that it comprises the entire $\overline{\Delta}_n$ yielding what we call the *extended Kolmogorov backward equation*

$$\begin{cases} -\frac{\partial}{\partial t}U(p, t) = L^*U(p, t) & \text{in } (\overline{\Delta}_n)_{-\infty} = \overline{\Delta}_n \times (-\infty, 0) \\ U(p, 0) = f(p) & \text{in } \overline{\Delta}_n, f \in \mathcal{L}^2(\bigcup_{k=0}^n \partial_k \Delta_n) \end{cases} \quad (5.1)$$

for $U(\cdot, t) \in C_p^2(\overline{\Delta}_n)$ for each fixed $t \in (-\infty, 0)$ and $U(p, \cdot) \in C^1((-\infty, 0))$ for each fixed $p \in \overline{\Delta}_n$. Here, f is the *extended final condition* which is defined on $\overline{\Delta}_n$. Thus, any boundary instance of the boundary of the simplex may also belong to the target set considered.

Our problem now is different from standard final-boundary value problems, because for such a solution, the configuration on the boundary is no longer static in general, but is governed by L_k^* with k being the corresponding dimension resp. by L_n^* restricted to the corresponding domain, matching the degeneracy behaviour of L_n^* (cf. lemma 3.3). Hence, the index may be omitted, and we may just write L^* (for dimension 0, we formally put $L^* = L_0^* := 0$ there). In terms of the underlying Wright–Fisher model, this signifies that the boundary is subject to the same type of evolution, merely in a different dimension, justifying the choice of equation (3.1).

The key point now is to connect the different boundary strata, by requiring $U \in C_p^2(\overline{\Delta}_n)$ w. r. t. the spatial variables: Clearly, inside each boundary instance the solution needs to be sufficiently regular for L^* , but regarding the boundary, we also demand such regularity for simple boundary transitions, i. e. when the dimension decreases by one. For higher order transitions, however, irregularities are admitted. This corresponds to the degeneracy behaviour of the operator at the boundary and will be observed with the solutions constructed. This allows for a much wider class of global solutions. These solutions are not artificial, but correspond to natural scenarios in the underlying Wright–Fisher model.

6 An extension scheme for solutions of the Kolmogorov backward equation

We want to construct the class of global solutions of the Kolmogorov backward equation (3.1) by successive backward extension of local solutions in different boundary strata. For this, we first look at single extensions of solutions from a boundary instance of the considered domain to the interior. The extensions are confined by:

6.1 Definition (extension constraints). Let I_d be an index set with $|I_d| = d + 1 \geq 2$, $0, s \in I_d$ and $\Delta_d^{(I_d)} = \{(p^i)_{i \in I_d \setminus \{0\}} | p^i > 0 \text{ for } i \in I_d\}$ with $p^0 := 1 - \sum_{i \in I_d \setminus \{0\}} p^i$. For $d \geq 2$ and a solution $u: (\Delta_{d-1}^{(I_d \setminus \{s\})})_{-\infty} \rightarrow \mathbb{R}$ of the Kolmogorov backward equation (3.1), i. e. $u(\cdot, t) \in C^\infty(\Delta_{d-1}^{(I_d \setminus \{s\})})$ for $t < 0$, $u(p, \cdot) \in C^\infty((-\infty, 0))$ for $p \in \Delta_{d-1}^{(I_d \setminus \{s\})}$ and

$$-\frac{\partial}{\partial t} u = L^* u \quad \text{in } (\Delta_{d-1}^{(I_d \setminus \{s\})})_{-\infty}, \quad (6.1)$$

a function $\bar{u}: (\Delta_d^{(I_d)})_{-\infty} \rightarrow \mathbb{R}$ with $\bar{u}(\cdot, t) \in C^\infty(\Delta_d^{(I_d)})$ for $t < 0$ and $\bar{u}(p, \cdot) \in C^\infty((-\infty, 0))$ for $p \in \Delta_d^{(I_d)}$ is said to be an extension of u in accordance with the *extension constraints* if

- (i) for $t < 0$ $\bar{u}(\cdot, t)$ is continuously extendable to the boundary $\partial_{d-1} \Delta_d^{(I_d)}$ such that it coincides with $u(\cdot, t)$ in $\Delta_{d-1}^{(I_d \setminus \{s\})}$ resp. vanishes on the remainder of $\partial_{d-1} \Delta_d^{(I_d)}$ and is of class C^∞ with respect to the spatial variables in $\Delta_d^{(I_d)} \cup \partial_{d-1} \Delta_d^{(I_d)}$,
- (ii) it is a solution of the corresponding Kolmogorov backward equation in $(\Delta_d^{(I_d)})_{-\infty}$, i. e. $-\frac{\partial}{\partial t} \bar{u} = L^* \bar{u}$ in $(\Delta_d^{(I_d)})_{-\infty}$.

For $d = 1$, this analogously applies to functions u with $-\frac{\partial}{\partial t} u = 0$ (in accordance with $L_0^* \equiv 0$), and consequently the equation in condition (ii) is replaced with $L^* \bar{u} = 0$. Furthermore, an extension which encompasses multiple extension steps is said to be in accordance with the extension constraints, if this holds for every extension step.

6.2 Remark. In case of $d \geq 2$, if u for $t < 0$ extends smoothly to the boundary $\partial_{d-2} \Delta_{d-1}^{(I_d \setminus \{s\})}$ such that this extension vanishes everywhere on $\partial_{d-2} \Delta_{d-1}^{(I_d \setminus \{s\})}$, the above definition corresponds to $(u \chi_{\Delta_{d-1}^{(I_d \setminus \{s\})}} + \bar{u} \chi_{\Delta_d^{(I_d)}}) \in C_{p_0}^\infty(\Delta_{d-1}^{(I_d \setminus \{s\})} \cup \Delta_d^{(I_d)})$ with respect to the spatial variables for $t < 0$ (cf. equality (2.13)) except for the Kolmogorov backward equation solution property.

We shall investigate here the existence of such extensions which comply with definition 6.1; the issue of their uniqueness will be dealt with in another paper. Corresponding to the chosen separation ansatz (on which the result 4.1 is based), we shall have to construct extensions of the eigenmodes:

6.3 Lemma (extension of eigenfunctions). *Let I_d be an index set with $|I_d| = d + 1 \geq 2$, $0, s \in I_d$ and $\Delta_d^{(I_d)} = \{(p^i)_{i \in I_d \setminus \{0\}} | p^i > 0 \text{ for } i \in I_d\}$ with $p^0 := 1 - \sum_{i \in I_d \setminus \{0\}} p^i$. For $d \geq 2$ and an eigenfunction $\psi \in C^\infty(\Delta_{d-1}^{(I_d \setminus \{s\})})$ of L_{d-1}^* for the eigenvalue $\kappa \geq 0$, i. e.*

$$L_{d-1}^* \psi = -\kappa \psi \quad \text{in } \Delta_{d-1}^{(I_d \setminus \{s\})} \subset \partial \Delta_d^{(I_d)}, \quad (6.2)$$

a linear interpolation $\bar{\psi} = \bar{\psi}^{r,s}: \Delta_d^{(I_d)} \rightarrow \mathbb{R}$ of ψ from $\Delta_{d-1}^{(I_d \setminus \{s\})}$ (source face) towards $\Delta_{d-1}^{(I_d \setminus \{r\})} \subset \partial_{d-1} \Delta_d^{(I_d)}$ for some $r \in I_d \setminus \{s\}$ (target face) is given by

$$\bar{\psi}^{r,s}(p) := \psi(\pi^{r,s}(p)) \cdot \frac{p^r}{p^s + p^r} \quad \text{for } p \in \Delta_d^{(I_d)} \quad (6.3)$$

with $\pi^{r,s}(p^1, \dots, p^d) = (\tilde{p}^1, \dots, \tilde{p}^d)$ such that $\tilde{p}^s = 0$, $\tilde{p}^r = p^s + p^r$ and $\tilde{p}^i = p^i$ for $i \in I_d \setminus \{s, r\}$.

The regularity of $\bar{\psi}$ corresponds to that of ψ in $\Delta_d^{(I_d)}$ (i. e. it is of class C^∞) and satisfies

$$L_d^* \bar{\psi} = -\kappa \bar{\psi} \quad \text{in } \Delta_d^{(I_d)}. \quad (6.4)$$

Moreover, $\bar{\psi}$ extends smoothly to $\Delta_{d-1}^{(I_d \setminus \{s\})}$ and $\Delta_{d-1}^{(I_d \setminus \{r\})}$, and there we have

$$\bar{\psi}|_{\Delta_{d-1}^{(I_d \setminus \{s\})}} = \psi, \quad \bar{\psi}|_{\Delta_{d-1}^{(I_d \setminus \{r\})}} = 0. \quad (6.5)$$

If furthermore ψ extends smoothly to $\Delta_{d-2}^{(I_d \setminus \{s,q\})} \subset \partial_{d-2} \Delta_d^{(I_d \setminus \{s\})}$ for some $q \in I_d \setminus \{r, s\}$, then $\bar{\psi}$ likewise extends smoothly to $\Delta_{d-1}^{(I_d \setminus \{q\})}$. In particular, $\bar{\psi}$ satisfies the extension constraint 6.1 (i) if ψ extends smoothly to $\partial_{d-2} \Delta_{d-1}^{(I_d \setminus \{s\})} \setminus \Delta_{d-2}^{(I_d \setminus \{r,s\})}$ and vanishes there.

For $d = 1$, the preceding statements analogously hold for arbitrary $\psi: \Delta_0^{(I_1 \setminus \{s\})} \rightarrow \mathbb{R}$ as eigenfunction of $L_0^ \equiv 0$ for the eigenvalue 0; then, $\bar{\psi}$ is of class C^∞ in $\Delta_1^{(I_1)}$, and such an extension is always in accordance with the extension constraint 6.1 (i).*

Since the eigenfunctions are the building blocks for a solution scheme, the preceding lemma directly extends to solutions of the Kolmogorov backward equation:

6.4 Proposition (extension of solutions). *Let I_d be an index set with $|I_d| = d + 1 \geq 2$, $0, s \in I_d$ and $\Delta_d^{(I_d)} = \{(p^i)_{i \in I_d \setminus \{0\}} | p^i > 0 \text{ for } i \in I_d\}$ with $p^0 := 1 - \sum_{i \in I_d \setminus \{0\}} p^i$. For $d \geq 2$, a given final condition $f \in \mathcal{L}^2(\Delta_{d-1}^{(I_d \setminus \{s\})})$ and a given extension target face index $r \in I_d \setminus \{s\}$, a solution $u: (\Delta_{d-1}^{(I_d \setminus \{s\})})_{-\infty} \rightarrow \mathbb{R}$ of the Kolmogorov backward equation (3.1), $u(\cdot, t) \in C^\infty(\Delta_{d-1}^{(I_d \setminus \{s\})})$ for $t < 0$ and $u(p, \cdot) \in C^\infty((-\infty, 0))$ for $p \in \Delta_{d-1}^{(I_d \setminus \{s\})}$, may be extended to a function*

$$\bar{u} = \bar{u}^{r,s}: (\Delta_d^{(I_d)})_{-\infty} \rightarrow \mathbb{R} \quad (6.6)$$

with $\bar{u}(\cdot, t) \in C^\infty(\Delta_d^{(I_d)})$ for $t < 0$ and $\bar{u}(p, \cdot) \in C^\infty((-\infty, 0))$ for $p \in \Delta_d^{(I_d)}$ as well as satisfying

$$-\frac{\partial}{\partial t}\bar{u} = L^*\bar{u} \quad \text{in } (\Delta_d^{(I_d)})_{-\infty}. \quad (6.7)$$

Furthermore, for $t < 0$ $\bar{u}(\cdot, t)$ smoothly extends to the boundary in $\Delta_{d-1}^{(I_d \setminus \{s\})}$ with

$$\bar{u}(\cdot, t)|_{\Delta_{d-1}^{(I_d \setminus \{s\})}} = u, \quad \text{in particular } \bar{u}(\cdot, 0)|_{\Delta_{d-1}^{(I_d \setminus \{s\})}} = f|_{\Delta_{d-1}^{(I_d \setminus \{s\})}} \quad (6.8)$$

and in $\Delta_{d-1}^{(I_d \setminus \{r\})}$ with $\bar{u}(\cdot, t)|_{\Delta_{d-1}^{(I_d \setminus \{r\})}} = 0$. If furthermore $u(\cdot, t)$ for $q \in I_d \setminus \{r, s\}$ extends smoothly to $\Delta_{d-2}^{(I_d \setminus \{q, s\})} \subset \partial_{d-2}\Delta_d^{(I_d \setminus \{s\})}$ for some t , then $\bar{u}(\cdot, t)$ likewise extends smoothly to $\Delta_{d-1}^{(I_d \setminus \{q\})}$. In particular, \bar{u} satisfies the extension constraints 6.1 if $u(\cdot, t)$ extends smoothly to $\partial_{d-2}\Delta_{d-1}^{(I_d \setminus \{s\})} \setminus \Delta_{d-2}^{(I_d \setminus \{r, s\})}$ and vanishes there for $t < 0$.

For $d = 1$, the preceding analogously holds for functions $u: (\Delta_0^{(I_1 \setminus \{s\})})_{-\infty} \rightarrow \mathbb{R}$ with $u(p, \cdot) \in C^\infty((-\infty, 0))$ and $\frac{\partial}{\partial t}u = 0$; then, $\bar{u}(\cdot, t)$ is of class C^∞ in $\Delta_1^{(I_1)}$ for every t as well as $\bar{u}(p, \cdot) \in C^\infty((-\infty, 0))$ for $p \in \Delta_d^{(I_d)}$ with $\frac{\partial}{\partial t}\bar{u} = 0$, and equation (6.7) holds correspondingly. Furthermore, this extension always is in accordance with the extension constraints 6.1.

6.5 Remark. The extension of a solution of the Kolmogorov backward equation for a final condition $f \in \mathcal{L}^2(\Delta_{d-1}^{(I_d \setminus \{s\})})$ as in proposition 6.4 is also applicable for $t = 0$, yielding an analogously extended final condition $\bar{f} = \bar{f}^{r,s} \in \mathcal{L}^2(\Delta_d^{(I_d)})$. We then have $\bar{u}(\cdot, 0) \equiv \bar{f}$ in $\Delta_d^{(I_d)}$ by continuous extension as we have $u(\cdot, 0) = f$ in $\Delta_{d-1}^{(I_d \setminus \{s\})}$; however, for $d \geq 2$ this extension of f in general does not have the boundary regularity described due to the missing regularity of f (and hence in general does not satisfy the extension boundary constraint 6.1 (i)).

In addition to the preceding proposition, it should be noted that \bar{u} does not necessarily extend continuously to the entire $\bar{\Delta}_d$, in particular not to the remaining boundary parts of dimension $d - 2$ and less. This is due to the fact that on instances of $\partial_{d-2}\Delta_d^{(I_d)}$, which are shared boundaries of higher-dimensional faces of the simplex, continuous extensions from each of those faces may exist, but do not necessarily coincide.

Proof of lemma 6.3. The regularity assertion for $\bar{\psi}$ in $\Delta_d^{(I_d)}$ follows from the regularity of π and of the projection and from $\frac{p^r}{p^s+p^r}$ being of class C^∞ on $\Delta_d^{(I_d)}$. The boundary behaviour is similarly straightforward as $\pi^{r,s} = \text{id}$ and $\frac{p^r}{p^s+p^r} = 1$ on $\Delta_{d-1}^{(I_d \setminus \{s\})}$, whereas $\frac{p^r}{p^s+p^r} = 0$ on $\Delta_{d-1}^{(I_d \setminus \{r\})}$. Both boundary extensions are smooth in the sense described, which is again due to the regularity of the projection and of $\frac{p^r}{p^s+p^r}$ when approaching $\Delta_{d-1}^{(I_d \setminus \{s\})}$ resp. $\Delta_{d-1}^{(I_d \setminus \{r\})}$. Analogous considerations yield the assertion for other boundary faces of $\partial_{d-1}\Delta_d^{(I_d)}$: The projection $\pi^{r,s}$ maps $\partial_{d-1}\Delta_d^{(I_d)} \setminus (\Delta_{d-1}^{(I_d \setminus \{r\})} \cup \Delta_{d-1}^{(I_d \setminus \{s\})})$

smoothly onto $\partial_{d-2}\Delta_{d-1}^{(I_d \setminus \{s\})}$, which together with $\frac{p^r}{p^s + p^r}$ being of class C^∞ on $\partial_{d-1}\Delta_d^{(I_d)}$ (via $p^s + p^r > 0$) yields the stated regularity; the value of this boundary extension of $\bar{\psi}$ of course coincides with the one of the corresponding extension of ψ .

To prove equation (6.4), w.l.o.g. let $I_d = \{0, 1, \dots, d\}$; summation indices, however, run from 1 to d if nothing differing is stated. To begin with, we have

$$\begin{aligned} L_d^* \left(\psi(\pi^{r,s}(p)) \cdot \frac{p^r}{p^s + p^r} \right) &= (L_d^* \psi(\pi^{r,s}(p))) \frac{p^r}{p^s + p^r} \\ &\quad + \sum_{i,j} p^i (\delta_j^i - p^j) \left(\frac{\partial}{\partial p^i} \psi(\pi^{r,s}(p)) \right) \left(\frac{\partial}{\partial p^j} \frac{p^r}{p^s + p^r} \right) \\ &\quad + \frac{1}{2} \psi(\pi^{r,s}(p)) \sum_{i,j} p^i (\delta_j^i - p^j) \left(\frac{\partial}{\partial p^i} \frac{\partial}{\partial p^j} \frac{p^r}{p^s + p^r} \right). \end{aligned} \quad (6.9)$$

Next, we will show that the first summand equals $-\kappa \bar{\psi}$, whereas the two other summands vanish on $\Delta_d^{(I_d)}$.

For the first summand, we use $L_{d-1}^* \psi = -\kappa \psi$ in $\Delta_{d-1}^{(I_d \setminus \{s\})}$, which holds by assumption. To extend this statement to $\Delta_d^{(I_d)}$, the interplay of the projection needs to be analysed, for which several cases are distinguished. That is, for $s \neq 0$, $r = 0$, the projection $\pi^{0,s}$ yields $\tilde{p}^s = 0$ and $\tilde{p}^i = p^i$ for $i \in \{1, \dots, d\} \setminus \{s\}$, hence $\frac{\partial \tilde{p}^m}{\partial p^i} = \delta_i^m (1 - \delta_s^m)$, and we have

$$\begin{aligned} L_d^* \psi(\pi^{0,s}(p)) &= \frac{1}{2} \sum_{i,j} p^i (\delta_j^i - p^j) \frac{\partial}{\partial p^i} \frac{\partial}{\partial p^j} \psi(\pi^{0,s}(p)) \\ &= \frac{1}{2} \sum_{m,n} \sum_{i,j} p^i (\delta_j^i - p^j) \delta_i^m (1 - \delta_s^m) \delta_j^n (1 - \delta_s^n) \frac{\partial}{\partial \tilde{p}^m} \frac{\partial}{\partial \tilde{p}^n} \psi(\tilde{p}) \\ &= \frac{1}{2} \sum_{m,n \neq s} \tilde{p}^m (\delta_n^m - \tilde{p}^n) \frac{\partial}{\partial \tilde{p}^m} \frac{\partial}{\partial \tilde{p}^n} \psi(\tilde{p}) = L_{d-1}^* \psi(\tilde{p}) \equiv -\kappa \psi(\tilde{p}). \end{aligned} \quad (6.10)$$

If $s = 0$, $r \neq 0$ and hence $\Delta_{d-1}^{(I_d \setminus \{0\})} = \{(\tilde{p}^1, \dots, \tilde{p}^d) | \tilde{p}^i > 0 \text{ for } i = 1, \dots, d, \sum_{i=1}^d \tilde{p}^i = 1\}$, we have $\tilde{p}^i = p^i$ for $i \in \{1, \dots, d\} \setminus \{r\}$ and $\tilde{p}^r = p^r + p^0$, thus $\frac{\partial \tilde{p}^m}{\partial p^i} = \delta_i^m - \delta_r^m$. We get:

$$\begin{aligned} L_d^* \psi(\pi^{r,0}(p)) &= \frac{1}{2} \sum_{m,n} \sum_{i,j} p^i (\delta_j^i - p^j) (\delta_i^m - \delta_r^m) (\delta_j^n - \delta_r^n) \frac{\partial}{\partial \tilde{p}^m} \frac{\partial}{\partial \tilde{p}^n} \psi(\tilde{p}) \\ &= \frac{1}{2} \sum_{m,n} p^m (\delta_n^m - p^n) \frac{\partial}{\partial \tilde{p}^m} \frac{\partial}{\partial \tilde{p}^n} \psi(\tilde{p}) - \frac{1}{2} \sum_n \sum_i p^i (\delta_n^i - p^n) \frac{\partial}{\partial \tilde{p}^r} \frac{\partial}{\partial \tilde{p}^n} \psi(\tilde{p}) \\ &\quad - \frac{1}{2} \sum_m \sum_j p^m (\delta_j^m - p^m) \frac{\partial}{\partial \tilde{p}^r} \frac{\partial}{\partial \tilde{p}^n} \psi(\tilde{p}) + \frac{1}{2} \sum_{i,j} p^i (\delta_j^i - p^j) \frac{\partial^2}{(\partial \tilde{p}^r)^2} \psi(\tilde{p}) \\ &= \frac{1}{2} \sum_{m,n} p^m (\delta_n^m - p^n) \frac{\partial}{\partial \tilde{p}^m} \frac{\partial}{\partial \tilde{p}^n} \psi(\tilde{p}) - \frac{1}{2} \sum_n p^0 p^n \frac{\partial}{\partial \tilde{p}^r} \frac{\partial}{\partial \tilde{p}^n} \psi(\tilde{p}) \end{aligned}$$

$$-\frac{1}{2} \sum_m p^m p^0 \frac{\partial}{\partial \tilde{p}^m} \frac{\partial}{\partial \tilde{p}^r} \psi(\tilde{p}) + \frac{1}{2} p^0 (1 - p^0) \frac{\partial^2}{(\partial \tilde{p}^r)^2} \psi(\tilde{p}). \quad (6.11)$$

When replacing the remaining p -coordinates by \tilde{p} (except for p^0 , which is missing in $\Delta_{d-1}^{(I_d \setminus \{0\})}$) via $p^i = \tilde{p}^i - p^0 \delta_r^i$ for $i = \{1, \dots, d\}$, the expression transforms into:

$$\begin{aligned} L_d^* \psi(\pi^{r,0}(p)) &= \frac{1}{2} \sum_{m,n \neq r} \tilde{p}^m (\delta_n^m - \tilde{p}^n) \frac{\partial}{\partial \tilde{p}^m} \frac{\partial}{\partial \tilde{p}^n} \psi(\tilde{p}) + \frac{1}{2} \sum_{n \neq r} (-\tilde{p}^r + p^0) \tilde{p}^n \frac{\partial}{\partial \tilde{p}^r} \frac{\partial}{\partial \tilde{p}^n} \psi(\tilde{p}) \\ &\quad + \frac{1}{2} \sum_{m \neq r} \tilde{p}^m (-\tilde{p}^r + p^0) \frac{\partial}{\partial \tilde{p}^m} \frac{\partial}{\partial \tilde{p}^r} \psi(\tilde{p}) + \frac{1}{2} (\tilde{p}^r - p^0) (1 - \tilde{p}^r + p^0) \times \\ &\quad \frac{\partial^2}{(\partial \tilde{p}^r)^2} \psi(\tilde{p}) - \frac{1}{2} \sum_{n \neq r} p^0 \tilde{p}^n \frac{\partial}{\partial \tilde{p}^r} \frac{\partial}{\partial \tilde{p}^n} \psi(\tilde{p}) - \frac{1}{2} \sum_{m \neq r} \tilde{p}^m p^0 \frac{\partial}{\partial \tilde{p}^m} \frac{\partial}{\partial \tilde{p}^r} \psi(\tilde{p}) \\ &\quad - p^0 (\tilde{p}^r - p^0) \frac{\partial^2}{(\partial \tilde{p}^r)^2} \psi(\tilde{p}) + \frac{1}{2} p^0 (1 - p^0) \frac{\partial^2}{(\partial \tilde{p}^r)^2} \psi(\tilde{p}) \\ &= \frac{1}{2} \sum_{m,n} \tilde{p}^m (\delta_n^m - \tilde{p}^n) \frac{\partial}{\partial \tilde{p}^m} \frac{\partial}{\partial \tilde{p}^n} \psi(\tilde{p}) = L_{d-1}^* \psi(\tilde{p}) \equiv -\kappa \psi(\tilde{p}). \end{aligned} \quad (6.12)$$

The next-to-last equality is due to the fact that in $\Delta_{d-1}^{(I_d \setminus \{0\})}$ one coordinate is obsolete and consequently ψ is formulated in $d-1$ coordinates (which may be chosen freely). It is straightforward to show that, independently of the choice of the omitted coordinate r , we have $L_{d-1}^* = \frac{1}{2} \sum_{m,n \neq r} \tilde{p}^m (\delta_n^m - \tilde{p}^n) \frac{\partial}{\partial \tilde{p}^m} \frac{\partial}{\partial \tilde{p}^n}$ on $\Delta_{d-1}^{(I_d \setminus \{0\})}$.

Lastly, if $s \neq 0$, $r \neq 0$, the projection $\pi^{r,s}$ yields $\tilde{p}^s = 0$, $\tilde{p}^r = p^s + p^r$ and $\tilde{p}^i = p^i$ for the remaining indices, hence $\frac{\partial \tilde{p}^m}{\partial p^i} = \delta_i^m (1 - \delta_s^m) + \delta_r^m \delta_s^i$. Then we have:

$$\begin{aligned} L_d^* \psi(\pi^{r,s}(p)) &= \frac{1}{2} \sum_{i,j} p^i (\delta_j^i - p^j) \frac{\partial}{\partial p^i} \frac{\partial}{\partial p^j} \psi(\pi^{r,s}(p)) \\ &= \frac{1}{2} \sum_{\substack{m,n, \\ i,j}} p^i (\delta_j^i - p^j) (\delta_i^m (1 - \delta_s^m) + \delta_r^m \delta_s^i) (\delta_j^n (1 - \delta_s^n) + \delta_r^n \delta_s^j) \frac{\partial}{\partial \tilde{p}^m} \frac{\partial}{\partial \tilde{p}^n} \psi(\tilde{p}) \\ &= \frac{1}{2} \sum_{m,n \neq s} p^m (\delta_n^m - p^n) \frac{\partial}{\partial \tilde{p}^m} \frac{\partial}{\partial \tilde{p}^n} \psi(\tilde{p}) - \frac{1}{2} \sum_{n \neq s} p^s p^n \frac{\partial}{\partial \tilde{p}^r} \frac{\partial}{\partial \tilde{p}^n} \psi(\tilde{p}) \\ &\quad - \frac{1}{2} \sum_{m \neq s} p^m p^s \frac{\partial}{\partial \tilde{p}^m} \frac{\partial}{\partial \tilde{p}^r} \psi(\tilde{p}) + \frac{1}{2} p^s (1 - p^s) \frac{\partial^2}{(\partial \tilde{p}^r)^2} \psi(\tilde{p}). \end{aligned} \quad (6.13)$$

Replacing the p -coordinates works as shown in the preceding case, and thereupon we obtain

$$L_d^* \psi(\pi^{r,s}(p)) = \frac{1}{2} \sum_{m,n \neq s} \tilde{p}^m (\delta_n^m - \tilde{p}^n) \frac{\partial}{\partial \tilde{p}^m} \frac{\partial}{\partial \tilde{p}^n} \psi(\tilde{p}) = L_{d-1}^* \psi(\tilde{p}) \equiv -\kappa \psi(\tilde{p}), \quad (6.14)$$

thus in total

$$L_d^* \psi(\pi^{r,s}(p)) = L_{d-1}^* \psi(\tilde{p}) \equiv -\kappa \psi(\tilde{p}) = -\kappa \psi(\pi^{r,s}(p)) \quad (6.15)$$

for arbitrary r, s , which is the desired equality result for the first summand.

To show that the two remaining summands vanish, an analogous case-by-case analysis is necessary. If $s = 0, r \neq 0$, we have $\frac{p^r}{p^0+p^r} = \frac{p^r}{1-\sum_{l \neq r} p^l}$. Due to (remember $\frac{\partial \tilde{p}^m}{\partial p^i} = \delta_i^m - \delta_r^m$)

$$\frac{\partial}{\partial p^r} \psi(\pi^{r,0}(p)) = \sum_m \frac{\partial \tilde{p}^m}{\partial p^r} \frac{\partial}{\partial \tilde{p}^m} \psi(\tilde{p}) = 0, \quad (6.16)$$

the second summand equalling

$$\begin{aligned} \sum_{i \neq r} p^i \left(\frac{\partial}{\partial p^i} \psi(\pi^{r,0}(p)) \right) \underbrace{\sum_j (\delta_j^i - p^j) \left(\frac{\partial}{\partial p^j} \frac{p^r}{1 - \sum_{l \neq r} p^l} \right)}_{= (1 - \sum_{j \neq r} p^j) \frac{p^r}{(1 - \sum_{l \neq r} p^l)^2} - p^r \frac{1}{1 - \sum_{l \neq r} p^l}} &= 0 \end{aligned} \quad (6.17)$$

along with the third summand equalling

$$\begin{aligned} \frac{1}{2} \psi(\pi^{r,0}(p)) \sum_{i \neq r} \left(\sum_{j \neq r} p^i (\delta_j^i - p^j) \left(\frac{\partial}{\partial p^i} \frac{\partial}{\partial p^j} \frac{p^r}{1 - \sum_{l \neq r} p^l} \right) \right. \\ \left. - 2p^i p^r \left(\frac{\partial}{\partial p^i} \frac{\partial}{\partial p^r} \frac{p^r}{1 - \sum_{l \neq r} p^l} \right) \right) \\ = \frac{1}{2} \psi(\pi^{r,0}(p)) \sum_{i \neq r} \left(p^i (1 - \sum_{j \neq r} p^j) \frac{2p^r}{(1 - \sum_{l \neq r} p^l)^3} - 2p^i p^r \frac{1}{(1 - \sum_{l \neq r} p^l)^2} \right) = 0 \end{aligned} \quad (6.18)$$

vanish.

Similarly, if $s \neq 0, r = 0$, thus $\frac{p^0}{p^s+p^0} = \frac{1-\sum_l p^l}{1-\sum_{l \neq s} p^l}$ and again (with $\frac{\partial \tilde{p}^m}{\partial p^i} = \delta_i^m (1 - \delta_s^m)$)

$$\frac{\partial}{\partial p^s} \psi(\pi^{0,s}(p)) = \sum_m \frac{\partial \tilde{p}^m}{\partial p^s} \frac{\partial}{\partial \tilde{p}^m} \psi(\tilde{p}) = 0, \quad (6.19)$$

the second summand equalling

$$\begin{aligned} \sum_{i \neq s} p^i \left(\frac{\partial}{\partial p^i} \psi(\pi^{0,s}(p)) \right) \underbrace{\sum_j (\delta_j^i - p^j) \left(\frac{\partial}{\partial p^j} \frac{1 - \sum_l p^l}{1 - \sum_{l \neq s} p^l} \right)}_{= (1 - \sum_j p^j) \frac{-1}{1 - \sum_{l \neq s} p^l} + (1 - \sum_{j \neq s} p^j) \frac{1 - \sum_l p^l}{(1 - \sum_{l \neq s} p^l)^2}} &= 0 \end{aligned} \quad (6.20)$$

vanishes, and the third summand via

$$\begin{aligned}
& \sum_{i,j} p^i (\delta_j^i - p^j) \frac{\partial}{\partial p^i} \frac{\partial}{\partial p^j} \frac{1 - \sum_l p^l}{1 - \sum_{l \neq s} p^l} \\
&= \sum_{i,j} p^i (\delta_j^i - p^j) \left(\frac{(\delta_s^i - 1) + (\delta_s^j - 1)}{(1 - \sum_{l \neq s} p^l)^2} + 2(1 - \delta_s^i)(1 - \delta_s^j) \frac{1 - \sum_l p^l}{(1 - \sum_{l \neq s} p^l)^3} \right) \\
&= -2 \frac{(\sum_{i \neq s} p^i)(1 - \sum_{j \neq s} p^j)}{(1 - \sum_{l \neq s} p^l)^2} + 2 \left(\sum_{i \neq s} p^i \right) \left(1 - \sum_{j \neq s} p^j \right) \frac{1 - \sum_l p^l}{(1 - \sum_{l \neq s} p^l)^3} = 0 \quad (6.21)
\end{aligned}$$

also does.

Ultimately, if $s \neq 0$, $r \neq 0$, we have

$$p^j \frac{\partial}{\partial p^j} \frac{p^r}{p^s + p^r} = \frac{p^s p^r}{(p^s + p^r)^2} (\delta_r^j - \delta_s^j). \quad (6.22)$$

Using this property for the second summand, we obtain

$$\begin{aligned}
& \sum_{i,j} p^i (\delta_j^i - p^j) \left(\frac{\partial}{\partial p^i} \psi(\pi^{r,s}(p)) \right) \left(\frac{\partial}{\partial p^j} \frac{p^r}{p^s + p^r} \right) \\
&= \sum_i \left(\frac{\partial}{\partial p^i} \psi(\pi^{r,s}(p)) \right) p^i \left(\sum_j \delta_j^i \left(\frac{\partial}{\partial p^j} \frac{p^r}{p^s + p^r} \right) - \sum_j p^j \left(\frac{\partial}{\partial p^j} \frac{p^r}{p^s + p^r} \right) \right) \\
&= \sum_i \frac{\partial}{\partial p^i} \psi(\pi^{r,s}(p)) \frac{p^s p^r}{(p^s + p^r)^2} (\delta_r^i - \delta_s^i) = 0. \quad (6.23)
\end{aligned}$$

The last equality is due to the fact that the sum over i in the last line vanishes in conjunction with the symmetry of π in the coordinates p^s and p^r , i.e. we have $\frac{\partial \bar{p}^m}{\partial p^i} = \delta_i^m (1 - \delta_s^m) + \delta_r^m \delta_s^i$ and consequently

$$\frac{\partial}{\partial p^s} \psi(\pi^{r,s}(p)) = \frac{\partial}{\partial \bar{p}^r} \psi(\bar{p}) = \frac{\partial}{\partial p^r} \psi(\pi^{r,s}(p)). \quad (6.24)$$

For the third summand, we use

$$\frac{\partial}{\partial p^i} \frac{\partial}{\partial p^j} \frac{p^r}{p^s + p^r} = 2 \frac{\delta_j^i (\delta_s^i p^r - \delta_r^i p^s)}{(p^s + p^r)^3} + \frac{\delta_s^i \delta_r^j (1 - \delta_j^i) (p^r - p^s)}{(p^s + p^r)^3} \quad (6.25)$$

and thereon get

$$\sum_{i,j} p^i (\delta_j^i - p^j) \frac{\partial}{\partial p^i} \frac{\partial}{\partial p^j} \frac{p^r}{p^s + p^r} = \frac{2p^s(1 - p^s)p^r - 2p^r(1 - p^r)p^s - 2p^s p^r (p^r - p^s)}{(p^s + p^r)^3} = 0. \quad (6.26)$$

Altogether, we have

$$L_d^* \bar{\psi} = L_d^* \left(\psi(\pi^{r,s}(p)) \cdot \frac{p^r}{p^s + p^r} \right) = -\kappa \psi(\pi^{r,s}(p)) \frac{p^r}{p^s + p^r} = -\kappa \bar{\psi} \quad (6.27)$$

for arbitrary $r, s \in I_d$, thus proving equation (6.4). \square

7 A probabilistic interpretation of the extension scheme

We shall now discuss the meaning of the extension constraints 6.1. A target set on the space of $d - 1$ alleles can not only be reached from a constellation of $d - 1$ alleles, but also from one of d alleles by allele loss. Therefore, we need to analyze how the attraction of such a target set also extends to the space of d alleles. A natural assumption for such an extension is that the probability density at the transition from the d -allelic domain to the $(d - 1)$ -allelic domain stays regular, i.e. small alterations of the allelic configuration should only affect the probability in a controlled way. This is formulated in condition (i) and implies the C_p^∞ regularity (cf. equality 2.12) for the corresponding domains. Moreover, a boundary condition enters, as for transitions to domains of a different set of $d - 1$ alleles, the corresponding probability should also stay regular with the additional requirement that in the limit it vanishes on those other $(d - 1)$ -allelic domains; this is also part of condition (i) and correspondingly implies the $C_{p_0}^\infty$ regularity (cf. equality 2.13). As a possible extension is so far only confined towards the boundary of the domain, we also wish to link the evolution of the original probability density and its extension by requiring that both are subject to the same type of evolution in the corresponding domain, i.e. are governed by the corresponding Kolmogorov backward equation in the relevant formulation, which is condition (ii).

The extension proposition 6.4 then states that any (proper) solution of the Kolmogorov backward equation, which describes the evolving attraction of some target set given via the final condition f , may be extended to a corresponding solution of the Kolmogorov backward equation in the domain of subsequent higher dimension with both conditions above applying. In the context of a Wright–Fisher model, this loss of the extra allele s is modelled as if it was in competition with just one other allele r dependent on the index chosen (*fibration property*). Thus, we say that allele s is lost over allele r .

However, as may be observed by remark 6.5, this extension actually yields the solution to a somewhat altered problem, namely the attraction generated by the target set itself plus an induced (generalised) target set in the bigger domain which are given by f and its corresponding extension \bar{f} . If one wishes to return to the original problem, the attraction of the original target set only located in the $(d - 1)$ -allelic domain, the induced target set needs to be compensated for by a proper solution in (the interior of) the d -allelic domain for a corresponding final condition.

As may also be seen in proposition 6.4, for $d \geq 2$ the given extension scheme involves a potential ambiguity regarding the choice of the extension target face index r . However, in case of iterations, the boundary condition in definition 6.1 (i) limits this to a unique appropriate value as will be demonstrated in the next section; for a simple extension from a 0-dimensional domain or if the starting distribution smoothly vanishes towards all boundaries of subsequent lower dimension (as with proper solutions), an extension is always in accordance with the boundary condition.

8 Iterated extensions

A repeated application of proposition 6.4 yields the existence of iterated extensions (generalising the corresponding result for $n = 2$ in [26] and the (less explicit) result stated in [28] without derivation):

8.1 Proposition (pathwise extension of solutions). *Let $k, n \in \mathbb{N}$ with $0 \leq k < n$, $\{i_k, i_{k+1}, \dots, i_n\} \subset I_n := \{0, 1, \dots, n\}$ with $i_i \neq i_j$ for $i \neq j$ and $I_k := I_n \setminus \{i_{k+1}, \dots, i_n\}$, and let u_{I_k} be a proper solution of the Kolmogorov backward equation (5.1) in $\Delta_k^{(I_k)}$ for some final condition $f \in \mathcal{L}^2(\Delta_k^{(I_k)})$ as in proposition 4.1. For $d = k+1, \dots, n$ and $I_d := I_k \cup \{i_{k+1}, \dots, i_d\}$, an extension of $\bar{u}_{I_k}^{i_k, \dots, i_{d-1}}$ in $(\Delta_{d-1}^{(I_{d-1})})_{-\infty}$ to $\bar{u}_{I_k}^{i_k, \dots, i_d} := (\bar{u}_{I_k}^{i_k, \dots, i_{d-1}})^{i_{d-1}, i_d}$ in $(\Delta_d^{(I_d)})_{-\infty}$ as by proposition 6.4 is in accordance with the extension constraints 6.1 if (and for $d \geq k+2$ and $[f] \neq 0$ in $L^2(\Delta_k^{(I_k)})$ also only if) putting $r(d) = i_{d-1}$ for the extension target face index, and we respectively have*

$$\bar{u}_{I_k}^{i_k, \dots, i_d}(p, t) = u_{I_k}(\pi^{i_k, \dots, i_d}(p), t) \prod_{j=k}^{d-1} \frac{p^{i_j}}{\sum_{l=j}^d p^{i_l}}, \quad (p, t) \in (\Delta_d^{(I_d)})_{-\infty} \quad (8.1)$$

with $p^0 = 1 - \sum_{i \in I_d \setminus \{0\}} p^i$ and $\pi^{i_k, \dots, i_d}(p) = (\tilde{p}^1, \dots, \tilde{p}^n)$ such that $\tilde{p}^{i_k} = p^{i_k} + \dots + p^{i_d}$, $\tilde{p}^{i_{k+1}} = \dots = \tilde{p}^{i_d} = 0$ and $\tilde{p}^j = p^j$ for $j \in I_d \setminus \{i_k, \dots, i_d\}$.

Correspondingly, the resulting assembling of all extensions to a function $\bar{U}_{I_k}^{i_k, \dots, i_n}$ in $(\bigcup_{k \leq d \leq n} \Delta_d^{(I_d)})_{-\infty}$ by putting

$$\begin{aligned} \bar{U}_{I_k}^{i_k, \dots, i_n}(p, t) &:= u_{I_k}(p, t) \chi_{\Delta_k^{(I_k)}}(p) + \sum_{k+1 \leq d \leq n} \bar{u}_{I_k}^{i_k, \dots, i_d}(p, t) \chi_{\Delta_d^{(I_d)}}(p) \\ &= u_{I_k}(p, t) \chi_{\Delta_k^{(I_k)}}(p) + \sum_{k+1 \leq d \leq n} u_{I_k}(\pi^{i_k, \dots, i_d}(p), t) \prod_{j=k}^{d-1} \frac{p^{i_j}}{\sum_{l=j}^d p^{i_l}} \chi_{\Delta_d^{(I_d)}}(p) \end{aligned} \quad (8.2)$$

with $p^0 = 1 - \sum_{i \in I_n \setminus \{0\}} p^i$ is in $C_{p_0}^\infty(\bigcup_{k \leq d \leq n} \Delta_d^{(I_d)})$ with respect to the spatial variables for $t < 0$ as well as in $C^\infty((-\infty, 0))$ with respect to t , and we have

$$\begin{cases} L^* \bar{U}_{I_k}^{i_k, \dots, i_n} = -\frac{\partial}{\partial t} \bar{U}_{I_k}^{i_k, \dots, i_n} & \text{in } (\bigcup_{k \leq d \leq n} \Delta_d^{(I_d)})_{-\infty} \\ \bar{U}_{I_k}^{i_k, \dots, i_n}(\cdot, 0) = \bar{F}_{I_k}^{i_k, \dots, i_n} & \text{in } \bigcup_{k \leq d \leq n} \Delta_d^{(I_d)} \end{cases} \quad (8.3)$$

with $\bar{F}_{I_k}^{i_k, \dots, i_n} \in \mathcal{L}^2(\bigcup_{k \leq d \leq n} \Delta_d^{(I_d)})$ being an analogous extension of the final condition $f = f_{I_k}$ in $\Delta_k^{(I_k)}$ as by remark 6.5; in particular, we have $\bar{U}_{I_k}^{i_k, \dots, i_n}|_{\Delta_k^{(I_k)}}(\cdot, 0) = f$ in $\Delta_k^{(I_k)}$.

8.2 Corollary. *For $n \in \mathbb{N}_+$, $k = 0$ and $u_{\{i_0\}} \equiv 1$ in $\Delta_0^{\{i_0\}} \subset \partial_0 \Delta_n$, equation (8.1) resp. equation (8.2) restricted to Δ_n and with the t -coordinate suppressed coincides with*

Littler's formula in Δ_n (cf. [28]):

$$\bar{U}_{\{i_0\}}^{i_0, i_1, \dots, i_n} \big|_{\Delta_n}(p) \equiv \bar{u}_{\{i_0\}}^{i_0, i_1, \dots, i_n}(p) = p^{i_0} \cdot \frac{p^{i_1}}{1 - p^{i_0}} \cdot \dots \cdot \frac{p^{i_{n-1}}}{1 - \sum_{l=0}^{n-2} p^{i_l}}. \quad (8.4)$$

Proof of proposition 8.1. The result is basically an application of proposition 6.4, which yields the regularity and the solution property (cf. equation (8.3)) in every $\Delta_d^{(I_d)}$. It only remains to show inductively that the boundary behaviour in each extension step respects the extension constraints 6.1 as well as the formula (8.1).

Clearly, a proper solution u_{I_k} of the Kolmogorov backward equation in $(\Delta_k^{(I_k)})_{-\infty}$ as in proposition 4.1 satisfies equation (8.1) and is of class $C_0^\infty(\Delta_k^{(I_k)})$ w.r.t. the spatial variables for $t < 0$ (which in particular implies that it is smoothly extendable to $\partial_{k-1}\Delta_k^{(I_k)}$). Extending u_{I_k} to $(\Delta_{k+1}^{(I_{k+1})})_{-\infty}$ via proposition 6.4 with $s(k+1) = i_{k+1}$ and $r(k+1) = i_k$ yields a function $\bar{u}_{I_k}^{i_k, i_{k+1}}$ of type (8.1), which for $t < 0$ smoothly extends to all boundary faces $\partial_k\Delta_{k+1}^{(I_{k+1})}$ and vanishes there except for $\Delta_k^{(I_k)}$ (where it coincides with u_{I_k}) by the assumed boundary behaviour of u_{I_k} . We may thus assume that for $k < d-1 < n$ an assembled extension $\bar{U}_{I_k}^{i_k, \dots, i_{d-1}}$ (corresponding to equation (8.2)) in $C_{p_0}^\infty(\bigcup_{k \leq m \leq d-1} \Delta_m^{(I_m)})$ with respect to the spatial coordinates exists whose top-dimensional component $\bar{U}_{I_k}^{i_k, \dots, i_{d-1}} \big|_{(\Delta_{d-1}^{(I_{d-1})})_{-\infty}} =: \bar{u}_{I_k}^{i_k, \dots, i_{d-1}}$ satisfies equation (8.1).

We may then perform an extension of $\bar{u}_{I_k}^{i_k, \dots, i_{d-1}}$ in $(\Delta_{d-1}^{(I_{d-1})})_{-\infty}$ to $\bar{u}_{I_k}^{i_k, \dots, i_d}$ in $(\Delta_d^{(I_d)})_{-\infty}$ via proposition 6.4 with $s(d) = i_d$ and $r(d) = i_{d-1}$. By the assumed boundary behaviour of $\bar{u}_{I_k}^{i_k, \dots, i_{d-1}}$ (i.e. $\bar{U}_{I_k}^{i_k, \dots, i_{d-1}}$ being of class $C_{p_0}^\infty$), $\bar{u}_{I_k}^{i_k, \dots, i_d}$ smoothly extends to all boundary faces $\partial_{d-1}\Delta_d^{(I_d)} \setminus \Delta_{d-1}^{(I_{d-1})}$ and vanishes there except for $\Delta_{d-1}^{(I_{d-1})}$ (where it coincides with $\bar{u}_{I_k}^{i_k, \dots, i_{d-1}}$) for $t < 0$. By putting $r(d) = i_{d-1}$, this particularly also holds for $\Delta_{d-1}^{(I_{d-1}) \setminus \{i_{d-1}\}}$, which in turn would otherwise be violated if $f \neq 0$ almost everywhere as may be seen from the proof of proposition 6.4. Then, the boundary behaviour respects the extension constraints 6.1, and we correspondingly have $\bar{U}_{I_k}^{i_k, \dots, i_d} := \bar{U}_{I_k}^{i_k, \dots, i_{d-1}} + \bar{u}_{I_k}^{i_k, \dots, i_d} \chi_{\Delta_d^{(I_d)}} \in C_{p_0}^\infty(\bigcup_{k \leq m \leq d} \Delta_m^{(I_m)})$ w.r.t. the spatial variables for $t < 0$.

To show equation (8.1), we obtain for $\bar{u}_{I_k}^{i_k, \dots, i_d}$ by equation (6.3) when plugging in the formula (8.1) for $\bar{u}_{I_k}^{i_k, \dots, i_{d-1}}$

$$\begin{aligned} \bar{u}_{I_k}^{i_k, \dots, i_d}(p, t) &= \bar{u}_{I_k}^{i_k, \dots, i_{d-1}}(\pi^{i_{d-1}, i_d}(p), t) \frac{p^{i_{d-1}}}{p^{i_{d-1}} + p^{i_d}} \\ &= u_{I_k}(\pi^{i_k, \dots, i_{d-1}}(\pi^{i_{d-1}, i_d}(p)), t) \prod_{j=k}^{d-2} \frac{(\pi^{i_{d-1}, i_d}(p))^{i_j}}{\sum_{l=j}^{d-1} (\pi^{i_{d-1}, i_d}(p))^{i_l}} \frac{p^{i_{d-1}}}{p^{i_{d-1}} + p^{i_d}} \\ &= u_{I_k}(\pi^{i_k, \dots, i_d}(p), t) \prod_{j=k}^{d-1} \frac{p^{i_j}}{\sum_{l=j}^d p^{i_l}} \quad \text{in } (\Delta_d^{(I_d)})_{-\infty} \end{aligned} \quad (8.5)$$

as $(\pi^{i_{d-1}, i_d}(p))^{i_j} = p^{i_j}$ for $i_j = i_k, \dots, i_{d-2}$ and $(\pi^{i_{d-1}, i_d}(p))^{i_{d-1}} = p^{i_{d-1}} + p^{i_d}$. If some index i_j equals zero (w.l.o.g. $i_0 = 0$) corresponding to $(\pi^{i_{d-1}, i_d}(p))^0$, this expression gets replaced by $p^0 \in \Delta_d^{(I_d)}$ as we have $(\pi^{i_{d-1}, i_d}(p))^0 = 1 - \sum_{j=1}^{d-1} (\pi^{i_{d-1}, i_d}(p))^{i_j} = 1 - \sum_{j=1}^d p^{i_j} \equiv p^0$. Furthermore, $\pi^{i_k, \dots, i_{d-1}}(\pi^{i_{d-1}, i_d}(p)) = \pi^{i_k, \dots, i_d}(p)$ directly follows from the definitions, thus proving equation (8.1) for $\bar{u}_{I_k}^{i_k, \dots, i_d}$ in $\left(\bigcup_{k \leq m \leq d} \Delta_m^{(I_m)}\right)_{-\infty}$. \square

8.3 Remark. Geometrically, the choice of the extension target face indices $s(d) = i_d$ and $r(d) = i_{d-1}$ signifies that the extension source face $\Delta_{d-1}^{(\{i_0, \dots, i_{d-2}, i_{d-1}\})}$ and the target face $\Delta_{d-1}^{(\{i_0, \dots, i_{d-2}, i_d\})}$ are adjacent faces to the highest degree, as they share $d-1$ vertices (for $d \geq 2$). Furthermore, their intersection $\Delta_{d-2}^{(\{i_0, \dots, i_{d-2}\})}$ is the extension source face of the previous step.

Sticking to the preceding probabilistic interpretation, $\bar{u}_{I_k}^{i_k, i_{k+1}, \dots, i_n}$ depicts the iterated ‘attraction’ of an (analogously extended) target set in $\Delta_k^{(I_k)}$ along a corresponding *extension path* specified by i_k, \dots, i_n resp. the corresponding index sets $I_k \subset \dots \subset I_n$. Thus, $\bar{u}_{I_k}^{i_k, i_{k+1}, \dots, i_n}$ gives the total probability for all paths in $\bar{\Delta}_n$ starting in $\Delta_n^{(I_n)}$, passing through the (sub)simplices

$$\Delta_{n-1}^{(I_{n-1})} \longrightarrow \Delta_{n-2}^{(I_{n-2})} \longrightarrow \dots \longrightarrow \Delta_{k+1}^{(I_{k+1})} \longrightarrow \Delta_k^{(I_k)} \quad (8.6)$$

and reaching the eventual target set, which, in the setting of the Wright–Fisher model, corresponds to eventually losing $n-k$ of originally n alleles in such a manner that from dimension $n-1$ down to 0 exactly the allele sets

$$I_n \longrightarrow I_{n-1} \longrightarrow \dots \longrightarrow I_{k+1} \longrightarrow I_k \quad (8.7)$$

are present until reaching the eventual target set.

As depicted, these pathwise extensions are a consequence of the boundary condition of the extension constraints 6.1: On the one hand, there is only one allele which is lost at a certain time; on the other hand, as this loss is modelled as if it was in competition with just one other allele, the corresponding allele always is the one which is lost next. Thus allele i_d is lost over i_{d-1} ; merely in the last step, i.e. the loss of allele i_{k+1} , the index i_k determines which of the alleles in I_k is the one i_{k+1} is lost over. Other extensions which may likewise be constructed by the extension lemma 6.3 will not be considered here.

However, the corresponding extensions in proposition 8.1 are not satisfactory to the extent that they lack a global (pathwise) regularity property on the entire $\bar{\Delta}_n$, i.e. are not in C_p^∞ w.r.t. the spatial variables, as this applies only along the corresponding extension path. Outside this path, generally no continuous (or even smooth) extensions exist. This is caused by the incompatibilities involved by this construction (cf. also section 7): For example on $\Delta_{k+1}^{(\tilde{I}_{k+1})}$ with $\tilde{I}_{k+1} := I_k \cup \{\tilde{i}_k\}$ and $\tilde{i}_k \in I_n \setminus I_{k+1}$, a positive hit probability for the target set in $\Delta_k^{(I_k)}$ by a direct loss of allele \tilde{i}_k would exist, yet the considered solution necessarily vanishes on $\Delta_{k+1}^{(\tilde{I}_{k+1})}$ as this is a boundary face of $\Delta_{k+2}^{(I_{k+2})}$ outside the specified path.

This defect is overcome by mounting these extensions into a global solution covering all possible extensions paths, each one of them corresponding to a certain ordering of the indices in $I_n \setminus I_k$. As in the first extension step, the extension target face is not defined for a given extension path and a non-empty target set by the extension boundary condition (i) in definition 6.1 (except for $k = 0$; cf. proposition 8.1), correspondingly all indices in I_k may serve as target face index. This is taken into account by additionally summing over all possible first stage extensions and normalising, yielding in total:

8.4 Proposition (global extension of solutions). *Let $k, n \in \mathbb{N}$ with $0 \leq k < n$, $I_k \subset I_n := \{0, 1, \dots, n\}$ with $|I_k| = k + 1$, and let u_{I_k} be a proper solution of the Kolmogorov backward equation (5.1) in $\Delta_k^{(I_k)}$ for some final condition $f \in \mathcal{L}^2(\Delta_k^{(I_k)})$ as in proposition 4.1. Then an assembling of all pathwise extensions of u_{I_k} as by proposition 8.1 into a function $\bar{U}_{I_k} \in (\bar{\Delta}_n)_{-\infty}$ by putting²*

$$\begin{aligned} \bar{U}_{I_k}(p, t) &:= u_{I_k}(p, t) \chi_{\Delta_k^{(I_k)}}(p) \\ &+ \frac{1}{|I_k|} \sum_{i_k \in I_k} \sum_{k+1 \leq d \leq n} \sum_{i_{k+1} \in I_n \setminus I_k} \cdots \sum_{\substack{i_d \in I_n \setminus (I_k \cup \\ \{i_{k+1}, \dots, i_{d-1}\})}} \bar{u}_{I_k}^{i_k, \dots, i_d}(p, t) \chi_{\Delta_d^{(I_k \cup \{i_{k+1}, \dots, i_d\})}}(p) \end{aligned} \quad (8.8)$$

for $(p, t) \in (\bigcup_{I_k \subset I_d \subset I_n} \Delta_d^{(I_d)})_{-\infty}$ and $\bar{U}_{I_k}(p, t) := 0$ in the remainder of $(\bar{\Delta}_n)_{-\infty}$ is in $C_p^\infty(\bar{\Delta}_n)$ with respect to the spatial variables for $t < 0$ as well as in $C^\infty((-\infty, 0))$ with respect to t . Furthermore, \bar{U}_{I_k} is a solution of the corresponding Kolmogorov backward equation in $(\bar{\Delta}_n)_{-\infty}$ and for $t = 0$ matches an analogously assembled extension \bar{F}_{I_k} of $f = f_{I_k}$ in $\Delta_k^{(I_k)}$ as final condition in $\bar{\Delta}_n$ (cf. remark 6.5).

Proof. The asserted global regularity directly follows from properties of the applied extension scheme as stated in lemma 6.3 and proposition 8.1 and the construction of \bar{U}_{I_k} , which is such that potential discontinuities are ruled out by assembling all extensions along arbitrary paths. The solution property and the compliance with the analogously constructed final condition likewise straightforwardly extend from proposition 8.1. \square

Shifting again to the probabilistic interpretation, \bar{U}_{I_k} now depicts the full iterated ‘attraction’ of some eventual target set in $\Delta_k^{(I_k)}$ and its (successively) induced target sets in $\Delta_d^{(I_d)} \subset \bar{\Delta}_n$ with $I_d \supset I_k$, which may now be reached along arbitrary paths. Thus, \bar{U}_{I_k} gives the total probability for all paths from $\Delta_n^{(I_n)}$ to eventually $\Delta_k^{(I_k)}$ – with no assumptions on possible interstages made. In the setting of the Wright–Fisher model, this corresponds to eventually losing $n - k$ of previously n alleles irrespective of any order of loss.

Since \bar{U}_{I_k} represents the most general extension of a given solution u_{I_k} in $\Delta_k^{(I_k)}$ to $\bar{\Delta}_n$, the general solution scheme for solutions of the extended Kolmogorov backward equation (5.1) may now be developed.

²The last sum actually only comprises a single summand; this notation is used to illustrate the choice of the index i_d , however.

9 Construction of general solutions via the extension scheme

For a given final condition $f = \sum_{d=0}^n f_d \chi_{\partial_d \Delta_n} \in \mathcal{L}^2(\bigcup_{d=0}^n \partial_d \Delta_n)$, the following extension scheme allows us to construct a solution of the extended Kolmogorov backward equation (5.1) which captures the full dynamics of the process on the entire $(\overline{\Delta_n})_{-\infty}$. The main ingredient for this are the global extensions of a (proper) solution of the Kolmogorov backward equation in every instance of the domain as in proposition 8.4; these globally extended solutions are superposed in a way that eventually the given final condition is met in the entire $\overline{\Delta_n}$ (cf. also section 7 for a probabilistic interpretation).

Thus, first equation (5.1) is solved in each $(\Delta_0^{\{i_0\}})_{-\infty} \subset (\partial_0 \Delta_n)_{-\infty}$ for the final condition f_0 , and afterwards, these solutions are successively extended to $(\overline{\Delta_n})_{-\infty}$ by means of proposition 8.4, which analogously generates a successively extended final condition in $\overline{\Delta_n}$ for $t = 0$. Subsequently, a (proper) solution in each $(\Delta_1^{(I_1)})_{-\infty} \subset (\partial_1 \Delta_n)_{-\infty}$ for the final condition f_1 minus the extension of f_0 is determined, which is then successively extended to $(\overline{\Delta_n})_{-\infty}$ (again likewise generating an analogously extended final condition). This procedure is repeated until after finding a (proper) solution in $(\Delta_n)_{-\infty}$ an extended solution in the entire $(\overline{\Delta_n})_{-\infty}$ is determined.

A solution of the extended Kolmogorov backward equation (5.1) restricted to some $(\Delta_0^{\{i_0\}})_{-\infty} \subset (\partial_0 \Delta_n)_{-\infty}$ is – of course – trivial, i. e. $u_{\{i_0\}}(p, t) = f_0(p)$ for $(p, t) \in (\Delta_0^{\{i_0\}})_{-\infty}$, and by proposition 8.4 we obtain $\bar{U}_{\{i_0\}}$ as an extension to $(\overline{\Delta_n})_{-\infty}$. Summing over all $\Delta_0^{\{i_0\}}$ yields

$$\bar{U}_0 := \sum_{\{i_0\} \subset I_n} \bar{U}_{\{i_0\}} \quad \text{in } (\overline{\Delta_n})_{-\infty} \quad (9.1)$$

with \bar{U}_0 in $C_p^\infty(\overline{\Delta_n})$ with respect to the spatial variables as well as in $C^\infty((-\infty, 0))$ with respect to t and

$$\begin{cases} L^* \bar{U}_0 = -\frac{\partial}{\partial t} \bar{U}_0 & \text{in } (\overline{\Delta_n})_{-\infty} \\ \bar{U}_0(\cdot, 0) = \bar{F}'_0 & \text{in } \overline{\Delta_n} \end{cases} \quad (9.2)$$

with \bar{F}'_0 being a corresponding superposed global extension of all $f'_0 \equiv f_0$ in $\partial_0 \Delta_n$ as described above for the $u_{\{i_0\}}$ (cf. also remark 6.5), in particular we have $\bar{U}_0|_{\partial_0 \Delta_n}(\cdot, 0) = f_0$.

For the next step, proper solutions in $(\partial_1 \Delta_n)_{-\infty}$ are determined and likewise extended to $(\overline{\Delta_n})_{-\infty}$. However, as this extension procedure will be repeated for all d -dimensional instances of $(\Delta_n)_{-\infty}$ for $d = 1, \dots, n$, we directly assume that suitable solutions in $(\bigcup_{m=0}^{d-1} \partial_m \Delta_n)_{-\infty}$ already have successively been determined and extended to $(\overline{\Delta_n})_{-\infty}$. Thus $\sum_{m=0}^{d-1} \bar{U}_m$ solves the extended Kolmogorov backward equation (5.1) in $(\overline{\Delta_n})_{-\infty}$ and matches the final condition f for $t = 0$ in $\bigcup_{m=0}^{d-1} \partial_m \Delta_n$ (still, with $\bar{U}_0(\cdot, 0), \dots, \bar{U}_{d-1}(\cdot, 0)$ in $\overline{\Delta_n}$ respectively matching a corresponding superposed global extension \bar{F}'_m of the final condition f'_m in $\partial_m \Delta_n$ modified as below). Then, a proper solution u_{I_d} by proposition 4.1

in each $(\Delta_d^{(I_d)})_{-\infty} \subset (\partial_d \Delta_n)_{-\infty}$, $I_d \subset I_n$ is determined which matches the modified final condition

$$f'_d := f_d - \sum_{m=0}^{d-1} \bar{F}'_m|_{\partial_d \Delta_n} \quad \text{in } \partial_d \Delta_n, \quad (9.3)$$

correspondingly restricted to the relevant $\Delta_d^{(I_d)}$. For each I_d , the solution u_{I_d} is then extended to $(\bar{\Delta}_n)_{-\infty}$ via proposition 8.4 each leading to a function \bar{U}_{I_d} . Clearly, these extensions do not interfere with the solutions on lower dimensional entities by definition.

Summing over the extensions of all u_{I_d} , $I_d \subset I_n$, we obtain

$$\bar{U}_d := \sum_{I_d \subset I_n} \bar{U}_{I_d} \quad \text{in } (\bar{\Delta}_n)_{-\infty} \quad (9.4)$$

as the global extension of all (proper) solutions in $(\partial_d \Delta_n)_{-\infty}$. By proposition 8.4 and the linearity of the differential equation, \bar{U}_d is in $C_p^\infty(\bar{\Delta}_n)$ w.r.t. the spatial variables as well as in $C^\infty((-\infty, 0))$ with respect to t and solves the extended Kolmogorov backward equation and for $t = 0$ matches a corresponding superposed global extension \bar{F}'_d of the final condition f'_d in $\partial_d \Delta_n$, thus in particular $\bar{U}_d(\cdot, 0)|_{\partial_d \Delta_n} = f'_d$. Consequently, the sum of all up to now extended solutions also is in $C_p^\infty(\bar{\Delta}_n)$ w.r.t. the spatial variables as well as in $C^\infty((-\infty, 0))$ with respect to t and satisfies

$$\begin{cases} L^* \left(\sum_{m=0}^d \bar{U}_m \right) = -\frac{\partial}{\partial t} \left(\sum_{m=0}^d \bar{U}_m \right) & \text{in } (\bar{\Delta}_n)_{-\infty} \\ \left(\sum_{m=0}^d \bar{U}_m \right)|_{\bigcup_{m=0}^d \partial_m \Delta_n}(\cdot, 0) = f|_{\bigcup_{m=0}^d \partial_m \Delta_n} & \text{in } \bigcup_{m=0}^d \partial_m \Delta_n. \end{cases} \quad (9.5)$$

Repeating the preceding step successively one eventually arrives at $\sum_{m=0}^{n-1} \bar{U}_m$. For the remaining $(\Delta_n)_{-\infty}$, at last a (proper) solution $u_{I_n} =: \bar{U}_n$ by proposition 4.1 is determined matching the modified final condition

$$f'_n := f_n - \sum_{m=0}^{n-1} \bar{F}'_m|_{\Delta_n} \quad \text{in } \Delta_n. \quad (9.6)$$

Then the sum of all globally extended (proper) solutions in all instances of the domain

$$\bar{U} := \sum_{j=0}^n \bar{U}_j \quad (9.7)$$

is in $C_p^\infty(\bar{\Delta}_n)$ w.r.t. the spatial variables as well as in $C^\infty((-\infty, 0))$ with respect to t and satisfies

$$\begin{cases} L^* \bar{U} = -\frac{\partial}{\partial t} \bar{U} & \text{in } (\bar{\Delta}_n)_{-\infty} \\ \bar{U}(\cdot, 0) = f & \text{in } \bar{\Delta}_n, \end{cases} \quad (9.8)$$

thus is a solution of the extended Kolmogorov backward equation (5.1).

Altogether, we have the following existence result:

9.1 Theorem. *For a given final condition $f \in \mathcal{L}^2(\bigcup_{d=0}^n \partial_d \Delta_n)$, the extended Kolmogorov backward equation (3.1) corresponding to the n -dimensional Wright–Fisher model in diffusion approximation always allows a solution $\bar{U}: (\bar{\Delta}_n)_{-\infty} \rightarrow \mathbb{R}$ with $\bar{U}(\cdot, t) \in C_p^\infty(\bar{\Delta}_n)$ for each fixed $t \in (-\infty, 0)$ and $\bar{U}(p, \cdot) \in C^\infty((-\infty, 0))$ for each fixed $p \in \bar{\Delta}_n$.*

In a following paper, we will be able to show that for $f \in \mathcal{L}^2(\partial_0 \Delta_n)$ – and under some additional regularity assumptions – the solution obtained, i. e. \bar{U}_0 , also is the unique solution given the described extension scheme.

10 The stationary Kolmogorov backward equation

Asking for the long-term behaviour of the process, i. e. which alleles are eventually lost and in which order, leads us to a stationary version of the Kolmogorov backward equation; solutions thereof have already appeared implicitly in the preceding section as extensions of solutions in $\partial_0 \Delta_n$ since the corresponding operator L_0^* only possesses the eigenvalue 0.

Even with the extended setting presented in section 5 available, we at first consider some interior simplex Δ_n , (resp. the corresponding restriction of an extended solution). Then, for a solution in Δ_n , we may argue again that all eigenmodes of the solution corresponding to a positive eigenvalue vanish for $t \rightarrow -\infty$, while those corresponding to the eigenvalue zero are preserved. Thus, it may be shown that a solution of the Kolmogorov backward equation (3.1) in Δ_n converges uniformly to a solution of the corresponding *homogeneous or stationary Kolmogorov backward equation*

$$\begin{cases} L^*u(p) = 0 & \text{in } \Delta_n \\ u(p) = f(p) & \text{in } \partial\Delta_n \end{cases} \quad (10.1)$$

for $u \in C^2(\Delta_n)$ and with boundary condition f (which needs to be attained smoothly in a certain sense).

At first sight, this appears as a boundary value problem (for some suitably chosen boundary function f , assuring the uniqueness of a solution). However, as may be expected from the previous considerations, the role of the boundary here is different from usual boundary value problems and again requires some extra care: On the one hand, a proper solution in Δ_n always converges to the trivial stationary solution (i. e. constantly equalling 0), which is linked to the fact that their (continuous) extension to the boundary also vanishes at all negative times. On the other hand, any solution which extends to $\partial\Delta_n$ is already strongly constrained by the degeneracy behaviour of the differential operator if suitable regularity assumptions on the solution in $\bar{\Delta}_n$ (cf. also equality (2.12)) apply:

10.1 Lemma (stem lemma). *For a solution $u \in C^\infty(\Delta_n)$ of equation (10.1) with extension $U \in C_p^\infty(\bar{\Delta}_n)$, we have*

$$L^*U = 0 \quad \text{in } \bar{\Delta}_n. \quad (10.2)$$

Proof. The statement is proven iteratively: Assuming that we have $L_k^*U = 0$ for all $\Delta_k^{(I_k)} \subset \partial_k \Delta_n$, we show that this property extends to each $\Delta_{k-1}^{(I_{k-1})} \subset \partial_{k-1} \Delta_k^{(I_k)}$ for every $\Delta_k^{(I_k)}$, hence we obtain $L_{k-1}^*U = 0$ on $\partial_{k-1} \Delta_n$. A repeated application then yields equation (10.2).

W.l.o.g. let $\Delta_k^{(I_k)}$ and $\Delta_{k-1}^{(I_{k-1})} \subset \partial_{k-1} \Delta_k^{(I_k)}$ with $I_k \setminus I_{k-1} = \{i_k\}$. Then for the operator L_k^* in $\Delta_k^{(I_k)}$, we have

$$L_k^* = L_{k-1}^* + p^{i_k} \left(\sum_{i_j \in I_k \setminus \{0\}} (\delta_{i_k}^{i_j} - p^{i_j}) \frac{\partial}{\partial p^{i_j}} \frac{\partial}{\partial p^{i_k}} \right) \quad (10.3)$$

with L_{k-1}^* being the restriction of L_k^* to $\Delta_{k-1}^{(I_{k-1})}$.

Now, choosing some $p \in \Delta_{k-1}^{(I_{k-1})}$ and a sequence $(p_l)_{l \in \mathbb{N}}$ in $\Delta_k^{(I_k)}$ with $p_l \rightarrow p$ and applying the above formula to U at $p_l \in \Delta_k^{(I_k)}$, the big bracket is controlled by $p_l^{i_k} \rightarrow 0$ while approaching p and – with the derivatives of U inside being bounded on a closed neighbourhood of p because of the regularity of U – is continuous up to p . Likewise, all derivatives of U within $\Delta_{k-1}^{(I_{k-1})}$ are continuously matched by the corresponding ones in $\Delta_k^{(I_k)}$, thus $L_{k-1}^*(U(p_l))$ is also continuous up to the boundary in p (as the corresponding coefficients are, too). Hence, the whole expression is continuous up to the boundary in p with $L_{k-1}^*U(p) \equiv L_k^*U(p) = 0$, and since p was arbitrary, this applies to all of $\Delta_{k-1}^{(I_{k-1})}$. \square

Assuming the stated pathwise regularity, this confines the boundary values of U resp. f on $\partial \Delta_n = \bigcup_{k=0}^{n-1} \partial_k \Delta_n$ and correspondingly, equation (10.1) is rather restated as an *extended homogeneous* or *extended stationary Kolmogorov backward equation*³

$$\begin{cases} L^*U(p) = 0 & \text{in } \overline{\Delta_n} \setminus \partial_0 \Delta_n \\ U(p) = f(p) & \text{in } \partial_0 \Delta_n \end{cases} \quad (10.4)$$

for $U \in C_p^2(\overline{\Delta_n})$ with the only ‘free’ boundary values remaining the ones on the vertices $\partial_0 \Delta_n$. If we also assume global continuity of the solution, the values on $\partial_0 \Delta_n$, however, suffice as boundary information determining a solution uniquely. In such a case, a stationary solution and the stationary component of a global extension as in the preceding section also coincide:

10.2 Proposition. *A solution $U \in C_p^\infty(\overline{\Delta_n}) \cap C^0(\overline{\Delta_n})$ of the extended stationary Kolmogorov backward equation (10.4) for some boundary condition $f_0: \partial_0 \Delta_n \rightarrow \mathbb{R}$ is uniquely defined and coincides with (the projection of) a solution of the extended Kolmogorov backward equation (5.1) in $(\overline{\Delta_n})_{-\infty}$ to $\overline{\Delta_n}$ for a final condition $f \in \mathcal{L}^2(\bigcup_{d=0}^n \partial_d \Delta_n)$ with $f \equiv f_0 \chi_{\partial_0 \Delta_n}$ as by theorem 9.1. Furthermore, the space of solutions is spanned by p^1, \dots, p^n and 1.*

³As already stated, it is without effect whether $\partial_0 \Delta_n$ is added to the domain of definition of the differential equation or not. Although $\partial_0 \Delta_n$ has been included in equation (10.2), this is not done here for formal reasons.

10.3 Remark. The first assertion of the preceding statement resembles the more general proposition 4.2.1 in [6]: Using their terminology, the corners $\partial_0 \Delta_n$ correspond to the *terminal boundary* $\partial \Delta_{n_{ter}}$, while by construction, the entire boundary is cleanly met by L^* ; however, the considered function spaces are not completely identical.

Proof. The first assertion may be shown by a successive application of the maximum principle: In every instance of the domain $\Delta_k^{(I_k)} \subset \partial_k \Delta_n$ for all $1 \leq k \leq n$, the operator L^* is locally uniformly elliptic, and hence, $U|_{\Delta_k^{(I_k)}}$ is uniquely defined by its values on $\partial \Delta_k^{(I_k)}$ by virtue of the maximum principle. Applying this consideration successively for $\partial_0 \Delta_n, \dots, \partial_n \Delta_n = \Delta_n$ yields the desired global uniqueness.

Next, we will show that a final condition $f = \chi_{\Delta_0^{(\{i_0\})}}$ for some $i_0 \in I_n$ gives rise to an extended solution $\bar{U}(p, t) = \bar{U}(p) = p^{i_0}$ in $(\bar{\Delta}_n)_{-\infty}$ resp. $\bar{\Delta}_n$ proving the second assertion. With f as described, the extended solution (cf. theorem 9.1) is solely given by $\bar{U} \equiv \bar{U}_{i_0}$, i. e.

$$\begin{aligned} \bar{U}_{\{i_0\}}(p, t) &= u_{\{i_0\}}(p, t) \chi_{\Delta_0^{(\{i_0\})}}(p) \\ &+ \sum_{1 \leq d \leq n} \sum_{i_1 \in I_n \setminus \{i_0\}} \cdots \sum_{i_d \in I_n \setminus \{i_0, \dots, i_{d-1}\}} U_{\{i_0\}}^{i_0, \dots, i_d}(p, t) \chi_{\Delta_d^{(\{i_0, \dots, i_d\})}}(p) \end{aligned} \quad (10.5)$$

(cf. equation (8.8)). Considering an arbitrary $\Delta_d^{(I_d)} \subset \bar{\Delta}_n$, $I_d \subset I_n$, we obtain for the restriction of \bar{U}_{i_0} to $\Delta_d^{(I_d)}$ using equation (8.2)

$$\begin{aligned} \bar{U}_{\{i_0\}}(p, t)|_{\Delta_d^{(I_d)}} &= \sum_{i_1 \in I_d \setminus \{i_0\}} \cdots \sum_{\substack{i_d \in \\ I_d \setminus \{i_0, \dots, i_{d-1}\}}} U_{\{i_0\}}^{i_0, \dots, i_d}(p, t) \\ &= \sum_{i_1 \in I_d \setminus \{i_0\}} \cdots \sum_{\substack{i_d \in \\ I_d \setminus \{i_0, \dots, i_{d-1}\}}} u_{\{i_0\}}(\pi^{i_0, \dots, i_d}(p), t) \prod_{j=0}^{d-1} \frac{p^{i_j}}{\sum_{l=j}^d p^{i_l}} \end{aligned} \quad (10.6)$$

with $u_{\{i_0\}}(\pi^{i_0, \dots, i_d}(p), t) \equiv 1$ as $\pi^{i_0, \dots, i_d}(p) \in \Delta_0^{(\{i_0\})}$ for all $p \in \Delta_d^{(I_d)}$ and $u_{\{i_0\}} = f = 1$ in $(\Delta_0^{(\{i_0\})})_{-\infty}$ by assumption. Since we have $\sum_{l=0}^d p^{i_l} = 1$ in $\Delta_d^{(I_d)}$, we may replace the expression $\sum_{l=j}^d p^{i_l}$ by $1 - \sum_{l=0}^{j-1} p^{i_l}$ and rearrange the sum (by also suppressing the last sum as the index i_d does no longer occur), which yields altogether

$$\begin{aligned} \bar{U}_{\{i_0\}}(p, t)|_{\Delta_d^{(I_d)}} &= \\ p^{i_0} &\left(\sum_{\substack{i_1 \in \\ I_d \setminus \{i_0\}}} \frac{p^{i_1}}{1 - p^{i_0}} \cdots \left(\sum_{\substack{i_j \in \\ I_d \setminus \{i_0, \dots, i_{j-1}\}}} \frac{p^{i_j}}{1 - \sum_{l=0}^{j-1} p^{i_l}} \cdots \left(\sum_{\substack{i_{d-1} \in \\ I_d \setminus \{i_0, \dots, i_{d-2}\}}} \frac{p^{i_{d-1}}}{1 - \sum_{l=0}^{d-2} p^{i_l}} \right) \right) \right). \end{aligned} \quad (10.7)$$

As we have $\frac{p^{i_j} + \dots + p^{i_d}}{1 - \sum_{l=0}^{j-1} p^{i_l}} = 1$ for $j = d-1, \dots, 1$, the whole expression reduces to $\bar{U}_{\{i_0\}}(p, t)|_{\Delta_d^{(I_d)}} = p^{i_0}$. Since $\Delta_d^{(I_d)}$ was arbitrary, we obtain $\bar{U}_{\{i_0\}}(p, t) \equiv \bar{U}_{\{i_0\}}(p) = p^{i_0}$ in the entire $\bar{\Delta}_n$. \square

Regarding the probabilistic interpretation, the extended setting (10.4) also matches the considerations of section 5 as equation (10.4) may be viewed as the limit equation for $t \rightarrow -\infty$ of the extended Kolmogorov backward equation (5.1) (which may be shown as previously). This is also reflected in proposition 10.2: For $t \rightarrow -\infty$ and any solution, the only target sets with persisting attraction are of course the vertices (respectively corresponding to configurations of the model where all but one allele are extinct), and hence the stationary solutions match the stationary components of the global extensions as in theorem 9.1, which in turn result from a non-vanishing final condition in $\partial_0 \Delta_n$. Then, every $\Delta_0^{\{i\}} \subset \partial_0 \Delta_n$ may give rise to a solution (component) p^i – in particular yielding a positive target hit probability on the entire Δ_n for all times. However, it is still noted that even the stationary component of solutions as in theorem 9.1 may in principle be perceived as time-dependent and also describing the transitional attraction of target sets in the entire $\overline{\Delta}_n$ induced by a given ultimate target set in $\partial_0 \Delta_n$.

In total, proposition 10.2 under the given restrictions thus already yields a full description of the stationary model in the entire $\overline{\Delta}_n$. However, dropping the global continuity assumption, a much wider class of (stationary) solutions may be observed as described in the preceding section.

References

- [1] S. Amari, H. Nagaoka, Methods of information geometry, Translations of mathematical monographs; v. 191, American Mathematical Society, 2000
- [2] N. Ay, J. Jost, H. V. Lê, L. Schwachhöfer, Information geometry, monograph, to appear
- [3] G. J. Baxter, R. A. Blythe, A. J. McKane. Exact Solution of the Multi-Allelic Diffusion Model. *Mathematical Biosciences*, 209(1):124–170, 2007.
- [4] R. Bürger, The mathematical theory of selection, recombination, and mutation, John Wiley, 2000
- [5] C. L. Epstein, R. Mazzeo, Wright-Fisher diffusion in one dimension, *SIAM J. Math. Anal.* 42 (2010), 568–608
- [6] C. L. Epstein, R. Mazzeo, Degenerate diffusion operators arising in population biology, Princeton Univ. Press, 2013
- [7] S. N. Ethier, A class of degenerate diffusion processes occurring in population genetics, *Comm. Pure Appl. Math.* 29 (1976), 483–493
- [8] S. N. Ethier, R. C. Griffiths, The Transition Function of a Fleming-Viot Process, *Ann Probab* 21 (1993) 1571–1590.
- [9] S. N. Ethier, T. Kurtz, Markov processes: characterization and convergence, Wiley, 1986, 2005

- [10] S. N. Ethier, T. Nagylaki, Diffusion Approximations of Markov Chains with Two Time Scales and Applications to Population Genetics, *Advances in Applied Probability* 12 (1980), 14–49
- [11] W. J. Ewens, *Mathematical Population Genetics I. Theoretical Introduction*, Springer-Verlag New York Inc., Interdisciplinary Applied Mathematics, 2nd ed., 2004.
- [12] R. A. Fisher, *On the dominance ratio*, *Proc. Roy. Soc. Edinb.*, **42** (1922), 321–341.
- [13] R. C. Griffiths, A Transition Density Expansion for a Multi-Allele Diffusion Model, *Adv Appl Probab* 11 (1979) 310–325
- [14] R. C. Griffiths, Lines of descent in the diffusion approximation of neutral Wright-Fisher models. *Theoret Popn Biol* 17 (1980) 37–50
- [15] R. C. Griffiths, D. Spanó, Diffusion processes and coalescent trees, Chapter 15, pp. 358–375. In: *Probability and Mathematical Genetics, Papers in Honour of Sir John Kingman*. LMS Lecture Note Series 378. ed Bingham, N. H. and Goldie, C. M., Cambridge University Press, 2010
- [16] J. Hofrichter, On the diffusion approximation of Wright-Fisher models with several alleles and loci and its geometry, PhD thesis, University of Leipzig, 2014
- [17] J. Hofrichter, T. D. Tran, J. Jost. A hierarchical extension scheme for solutions of the Wright–Fisher model, submitted
- [18] J. Jost. *Partial Differential Equations*, volume 214 of *Graduate Texts in Mathematics*. Springer, Berlin, Heidelberg, 3rd edition, 2013.
- [19] J. Jost. *Mathematical methods in biology and neurobiology*, Universitext, Springer, London, Heidelberg, 2014
- [20] S. Karlin, H. M. Taylor, A second course in stochastic processes, Academic Press, 1981
- [21] M. Kimura, *Solution of a Process of Random Genetic Drift with a Continuous Model*, *PNAS–USA*, Vol. 41, No. 3, (1955), 144–150.
- [22] M. Kimura, *Random genetic drift in multi-allele locus*, *Evolution*, **9** (1955), 419–435.
- [23] M. Kimura, *Random genetic drift in a tri-allelic locus; exact solution with a continuous model*, *Biometrics*, **12** (1956), 57–66.
- [24] M. Kimura. Random Genetic Drift in a Tri-Allelic Locus; Exact Solution with a Continuous Model. *Biometrics*, 12(1):57–66, 1956.
- [25] J. F. C. Kingman, The coalescent, *Stoch Proc Appl* 13 (1982) 235–248

- [26] R. A. Littler. Loss of Variability at One Locus in a Finite Population. *Mathematical Biosciences*, 25(1-2):151–163, 1975.
- [27] R. A. Littler and E. D. Fackerell. Transition Densities for Neutral Multi-Allele Diffusion Models. *Biometrics*, 31(1):117–123, 1975.
- [28] R. A. Littler and A. J. Good. Ages, Extinction Times, and First Passage Probabilities for a Multiallele Diffusion Model with Irreversible Mutation. *Theoretical Population Biology*, 13(2):214–225, 1978.
- [29] B. Øksendal. *Stochastic Differential Equations*. Universitext. Springer, Berlin, Heidelberg, 6th edition, 2003.
- [30] K. Sato, Diffusion operators in population genetics and convergence of Markov chains, In Measure Theory Application to Stochastic Analysis, LNM 695 (1978) 127–137
- [31] N. Shimakura, Équations différentielles provenant de la génétique des populations, Tohoku Math J. 29 (1977) 287-318
- [32] N. Shimakura, Formulas for diffusion approximations of some gene frequency models, J Math Kyoto Univ 21 (1981) 19-45
- [33] Tavaré S., Line-of-descent and genealogical processes, and their applications in population genetics models, Theor Popn Biol 26 (1984) 119-164
- [34] T.D. Tran. *Information Geometry and the Wright-Fisher Model of Mathematical Population Genetics*. PhD thesis, University of Leipzig, 2012.
- [35] T.D. Tran, J. Hofrichter, J. Jost. An introduction to the mathematical structure of the Wright-Fisher model of population genetics, Theory Biosci. (2012), 1–10
- [36] T.D. Tran, J. Hofrichter, J. Jost. A general solution of the Wright-Fisher model of random genetic drift, submitted
- [37] T.D. Tran, J. Hofrichter, J. Jost. The evolution of moment generating functions for the Wright-Fisher model of population genetics, submitted
- [38] S. Wright, *Evolution in Mendelian populations*, Genetics, **16** (1931), 97-159.
- [39] S. Wright, Adaptation and selection. In: G.Jepson, E.Mayr, G.Simpson (eds.), Genetics, Paleontology, and Evolution, pp.365-389, Princeton Univ.Press, 1949